Quantum Notes

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I am starting these notes about halfway through the class. This is for the first semester of graduate quantum mechanics from Sakurai.

Contents

1 Heisenberg vs. Shrodinger

Outline:

- Heisenberg base kets (2.2 SAK).
- Harmonic Oscillator (2.3 SAK).

Review from last lecture.

Theorem 1.1 (Ehrenfest)**.** *For a particle in a potential*

$$m\frac{d^2\hat{x}}{dt^2} = -v'(\hat{x}) \tag{1.1}$$

So we we know that

$$A\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle \tag{1.2}$$

We can relate the Shrodinger and Haeisenberg ictures as

$$a^H(t) = U^\dagger(t)A^S U(t) \tag{1.3}$$

where A^H is the Heisenberg time evolution operator which acts as

$$A^H(t)\left|\alpha;t\right\rangle_H = \alpha\left|\alpha;t\right\rangle \tag{1.4}$$

which implies that

$$A^S U(t)U^\dagger(t)\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle \tag{1.5}$$

Since we know that $\left|\alpha;t\right\rangle_H = U^\dagger(t)\left|\alpha\right\rangle$ we then have

$$A^H(t)U^\dagger(t)\left|\alpha\right\rangle = \alpha U^\dagger(t)\left|\alpha\right\rangle \tag{1.6}$$

which implies that

$$\underbrace{U^\dagger(t)A^S U}_{A^H} U^\dagger\left|\alpha\right\rangle = \alpha\underbrace{U^\dagger\left|\alpha\right\rangle}_{\left|\alpha;t\right\rangle_H} \tag{1.7}$$

We can note that this obeys a Schrodinger like equation with a different sign of

$$i\hbar\partial_t\left|\alpha;t\right\rangle_H = -H\left|\alpha;t\right\rangle \tag{1.8}$$

We note that this new basis is a suitable orthonormal basis and we can show that

$$\begin{aligned} A^H(t) = U^\dagger(t)A^S U(t) \\ &= \sum_\alpha \alpha\left|\alpha;t\right\rangle_H \left\langle\alpha;t\right|_H \\ &= \sum_\alpha \alpha U^\dagger\left|\alpha\right\rangle\left\langle\alpha\right|U \\ &= U^\dagger(t)A^S U(t) \end{aligned} \tag{1.9}$$

1.1 Transition Amplitude

We start in some state $|\psi\rangle$ and we evolve in some time and ask

$$\langle\alpha|U(t)|\psi\rangle \quad \text{Schrodinger} \tag{1.10}$$

In the Heisenberg picture this is

$$_H\langle\alpha, H\psi\rangle \tag{1.11}$$

This is called the transition amplitude. This is not completely in Heisenberg picture because ψ is in the Schrodinger picture, but we can rewrite this as

$$_H\langle\alpha, t|\psi\rangle_H \tag{1.12}$$

We want to choose

$$|\psi\rangle_H = |\beta; t = 0\rangle_H \tag{1.13}$$

where β is an eigenvalue given as

$$B^H(t)\,|\beta; t\rangle = \beta\,|\beta; t'\rangle_H \tag{1.14}$$

So we can define the transition amplitude as

$$_H\langle\alpha; t|\beta; t'\rangle_H \tag{1.15}$$

We can relate this to the Schrodinger picture as

$$\left\langle\alpha|U(t)U^\dagger(t')|\beta\right\rangle = \langle\alpha|U(t-t')|\beta\rangle \tag{1.16}$$

So this tells us that the transition amplitude is also given in the Schrodinger picture as the probability of going from $|\beta\rangle \to |\alpha\rangle$ in time $t - t'$.
Note that the Heisenberg kets are really kets of the operator, not the system. So we are really talking about time evolution of operators. If we wanted to calculate some probability, we would need to insert a complete set of base kets as

$$_H\langle\alpha; t|\psi\rangle = \sum_B {}_H\langle\alpha; t|\beta; t'\rangle_H \, {}_H\langle\beta; t'|\psi\rangle \tag{1.17}$$

In summary, we have the following table

	S	H
State Kets	Y	N
Observables	N	Y
Base kets	N	Y
Expectation	S	S
Transition	S	S

Table 1: Comparison of Heisenberg and Schrodinger picture. Y and N state whether the quantities change. S means the two are the same in both pictures.

2 Quantum Harmonic Oscillator

This is a very important system. The Hamiltonian for a particle is given as

$$H = \frac{p^2}{2m} + V(x). \tag{2.1}$$

For the Harmonic oscillator, $V(x) = \dfrac{m\omega^2}{2}x^2$ which implies our Hamiltonian is given as

$$H_{SHM} = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2. \tag{2.2}$$

We want to define a rescaled p and x to get a more symmetric Hamiltonian. So choose

$$\tilde{p} = \frac{1}{\alpha}p \ ; \ \tilde{x} = \alpha x, \tag{2.3}$$

Note this does not change the commutation relation. We want

$$\frac{\alpha^2}{2m} = \frac{m\omega^2}{2\alpha^2} \tag{2.4}$$

which tells us that $\alpha = \sqrt{m\omega}$. This leads us to the rescaled Hamiltonian

$$H = (\tilde{p}^2 + \tilde{x}^2)\frac{\omega}{2}. \tag{2.5}$$

Define an operator

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) = \frac{\tilde{x} + i\tilde{p}}{\sqrt{2\hbar}} \tag{2.6}$$

which tells us that

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right), \tag{2.7}$$

where a is given by the above equation. Note that $[a, a^\dagger] = 1$. To wrtie down the eigenvalues of H, we need to notice that

$$H = \hbar\omega\left(\hat{N} + \frac{1}{2}\right) \tag{2.8}$$

where $\hat{N}$ is the number operator given by $a^\dagger a$ and it is easy to see that $\left\langle \hat{N} \right\rangle \geq 0$. If we compute the commutation relation, we have

$$\begin{aligned}[\hat{N}, a] &= [a^\dagger a, a] \\ &= [a^\dagger, a]a + a^\dagger[a, a] \\ &= -a \end{aligned} \tag{2.9}$$

So this tells us that

$$\begin{aligned}\hat{N}\left|n\right\rangle &= n\left|n\right\rangle \\ \hat{N}a\left|n\right\rangle &= (a\hat{N} + [\hat{N}, a])\left|n\right\rangle \\ &= (an - a)\left|n\right\rangle \end{aligned} \tag{2.10}$$

which implies that $a|n\rangle = |n-1\rangle$. (These $a, a^\dagger$ are sometimes called raising and lowering operators). The only way in which we can be consistent with this relation and the expectation value is if $n \in \mathbb{Z}_{\geq 0}$.
We can identify the creation operator as $a^\dagger$ and the annihilation operator as a. We can easily see that

$$H|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle, \tag{2.11}$$

which implies that $E_n = \hbar\omega(n+1/2)$. Now we want to find the eigenstates of this in real space. What is $\psi_n(x) = \langle x|n\rangle$? We know that

$$a|n\rangle \propto |n-1\rangle \implies \hat{n}(a|n\rangle) = (n-1)(a|n\rangle) \tag{2.12}$$

We have a proprtion here, we need to find the normalization factor so we have a normalized state. So

$$\begin{aligned} a|n\rangle &= \lambda|n-1\rangle \\ \implies |\lambda|^2\langle n-1|n-1\rangle &= \langle n|a^\dagger a|n\rangle \\ &= n\langle n|n\rangle \\ \implies \lambda &= \sqrt{n} \end{aligned} \tag{2.13}$$

So this implies that

$$a|n\rangle = \sqrt{n}|n-1\rangle. \tag{2.14}$$

Similarly, $a^\dagger$ needs to be normalized. By identifying with the number operator we have

$$aa^\dagger|n\rangle = \hat{N}|n\rangle = n|n\rangle \tag{2.15}$$

but also

$$a^\dagger a|n\rangle = a^\dagger\sqrt{n}|n-1\rangle = n|n\rangle, \tag{2.16}$$

which implies that

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{2.17}$$

This leads us to

$$\begin{aligned} |1\rangle &= \frac{1}{\sqrt{1}}a^\dagger|0\rangle \\ |2\rangle &= \frac{1}{\sqrt{2}}a^\dagger|1\rangle = \frac{(a^\dagger)^2}{2}|0\rangle \\ \implies |n\rangle &= \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \end{aligned} \tag{2.18}$$

So if we know $|0\rangle$, then we can find the rest of the states. So we want to find

$$\psi_0(x) = \langle x|0\rangle. \tag{2.19}$$

We already now that

$$\langle x'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\langle x'|x + ip/(m\omega)|0\rangle \tag{2.20}$$

This implies that

$$\langle x'|x|0\rangle + \frac{i}{m\omega}\langle x'|P|0\rangle = 0. \tag{2.21}$$

This is a differential equation, since we can write this as

$$x'\psi_0(x') + \frac{i}{m\omega}(-i\hbar\partial_{x'}\psi_0(x') = 0 \tag{2.22}$$

We can rewrite this as

$$\frac{\hbar}{m\omega}\frac{\partial}{\partial x'}\psi_0(x') = -x'\psi_0(x'), \tag{2.23}$$

which has a solution of

$$\psi_0(x') = Ae^{-m\omega(x')^2/(2\hbar)} \tag{2.24}$$

We can normalize to get $A = (\sqrt{\pi x_0})^-1$. and write this as

$$\psi_0(x) = \frac{1}{\pi^{1/2}\sqrt{x_0}}\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \tag{2.25}$$

To get the other states, we can simply apply the raising operator as

$$\psi_n(x') = \left\langle x'\left|\frac{(a^\dagger)^n}{\sqrt{n!}}\right|0\right\rangle \tag{2.26}$$

This leads us to

$$\begin{aligned}\left\langle x'|a^\dagger|\psi\right\rangle &= \sqrt{\frac{m\omega}{2\hbar}}\left\langle x'\left|\hat{x} - \frac{i}{m\omega}\hat{p}\right|\psi\right\rangle \\ &= \sqrt{\frac{m\omega}{2\hbar}}\left(x' - \frac{\hbar}{m\omega}\partial_{x'}\right)\psi(x').\end{aligned} \tag{2.27}$$

So formally, we can write the equation as

$$\psi_n(x') = \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{2\hbar}\right)^{n/2}\left(x' - \frac{\hbar}{2\omega}\partial_{x'}\right)^n\psi_0(x'), \tag{2.28}$$

which in principle will give you all the states. There is a result which says that

$$\psi_n(x) = A_1 H_n\left(\frac{x'}{x_0}A_2\right)e^{-(x')^2/(2x_0^2)} \tag{2.29}$$

where the A_i are normalization factors and H_n is a Hermite polynomial in x'.

2.1 Uncertainty of QHO

If we look at this in more detail, this result looks like a Gaussian wave packet. We can find that

$$\left\langle x^2\right\rangle = \frac{x_0^2}{2}. \tag{2.30}$$

To find the expectation value of p^2, we note that

$$\begin{aligned}\left(\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2\right)\omega_0(x)&=\frac{1}{2}\hbar\omega\psi_0(x)\\ \implies \frac{1}{2m}\left\langle p^2\right\rangle+\frac{m\omega^2}{2}\left\langle x^2\right\rangle&=\frac{1}{2}\hbar\omega\\ \implies \frac{1}{2m}\left\langle p^2\right\rangle&=\frac{\hbar\omega}{4},\end{aligned}\tag{2.31}$$

which implies that

$$\left\langle x^2\right\rangle\left\langle p^2\right\rangle=\frac{\hbar^2}{4},\tag{2.32}$$

which implies that the ground state of the quantum harmonic oscillator is a minimum uncertainty state. The minimal way to get to a more general proof which is that for $\psi_n(x)$

$$\left\langle x^2\right\rangle\left\langle p^2\right\rangle=(n+1/2)^2\hbar^2,\tag{2.33}$$

we use the Virial Theorem which relates the kinetic energy expectation value to the potential energy expectation value.

2.2 Time Evolution of QHO

We can sove the time evolution in the Heisenberg picture as

$$\frac{d\hat{x}}{dt}=\frac{\hat{p}}{m}\,;\,\frac{d\hat{p}}{t}=-m\omega^2\hat{x}.\tag{2.34}$$

We can now use hte evolution of the creation and anhillation oeprator to help understand this

$$\begin{aligned}\frac{d}{dt}\hat{a}&=-i\omega\hat{a}\\ \implies \hat{a}(t)&=e^{-i\omega t}\hat{a}(0).\end{aligned}\tag{2.35}$$

Since we know that

$$\frac{d}{dt}\hat{a}^\dagger=i\omega\hat{a}^\dagger\tag{2.36}$$

we have that

$$\hat{a}^\dagger(t)=e^{i\omega t}\hat{a}^\dagger(0).\tag{2.37}$$

Using these, we have that

$$\begin{aligned}\hat{x}(t)&=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}(t)+\hat{a}^\dagger(t)\right)\\ &=\sqrt{\frac{\hbar}{2m\omega}}\left(e^{-i\omega t}\hat{a}(0)+e^{i\omega t}\hat{a}^\dagger(0)\right)\\ &=\hat{x}(0)\cos(\omega t)+\frac{\hat{p}(0)}{m\omega}\sin(\omega t)\end{aligned}\tag{2.38}$$

Similiarly, we have that

$$\hat{p}(t)=\hat{p}(0)\cos(\omega t)-m\omega\hat{x}(0)\sin(\omega t).\tag{2.39}$$

Note that there seems to be a contradiction if $|\psi\rangle = |n\rangle$. Then we have that

$$\begin{aligned}(\langle n|\hat{p}|n\rangle)(t) &= \left\langle n|e^{i\hat{H}t/\hbar}\hat{p}e^{-i\hat{H}t/\hbar}|n\right\rangle \\ &= \langle n|\hat{p}|n\rangle\,, \end{aligned} \tag{2.40}$$

which is not a contradiction if the expectation value of the operators p, x are zero when $|\psi\rangle = |n\rangle$.

2.2.1 Campbell-Baker-Hausdorff Relation

We can expand a certain form of operator in a power series

$$e^{i\lambda G}Ae^{-i\lambda G} = A + i\lambda[G,A] + \frac{(i\lambda)^2}{2!}[G,[G,A]] + \frac{(i\lambda)^3}{3!}[G,[G,[G,A]]] + \ldots \tag{2.41}$$

While this may look rather messy, if $[G,A] = n$ where n is a number, then only the first two terms survive. If we write

$$\hat{x}(t) = \exp\left(\frac{i\hat{H}t}{\hbar}\right)\hat{x}(0)\exp\left(\frac{-i\hat{H}t}{\hbar}\right), \tag{2.42}$$

Then we know that

$$[\hat{H},\hat{x}(0)] = \frac{-i\hbar}{m}\hat{p}(0) \tag{2.43}$$

$$[\hat{H},\hat{p}(0)] = i\hbar\omega^2 m\hat{x}(0). \tag{2.44}$$

So we get that

$$[\hat{H}[\hat{H},\hat{x}(0)]] = \hbar^2\omega^2\hat{x}(0) \tag{2.45}$$

This implies that we can actually evaluate the power series as

$$\begin{aligned}\hat{x}(t) &= \hat{x}(0) + \frac{(i\lambda)^2}{2}[\hat{H},[\hat{H},\hat{x}(0)]] + \cdots + i\lambda[\hat{H},(x_0 + \frac{1}{3!}[\hat{H},[\hat{H},\hat{x}(0)](i\lambda)^2 + \ldots \\ &= \hat{x}(0)\left(1 + \frac{1}{2}\left(\frac{it}{\hbar}\right)^2 + \frac{1}{4!}\left(\frac{it}{\hbar}\right)^4 + \ldots\right) + \left[H,\hat{x}(0)\left(\left(\frac{it}{\hbar}\right) + \frac{1}{3!}\left(\frac{it}{\hbar}\right)^3(\hbar\omega^2 + \ldots\right)\right] \\ &= \hat{x}(0)\cos(\omega t) + \frac{1}{m\omega}\hat{p}(0)\sin(\omega t). \end{aligned} \tag{2.46}$$

This agrees with our previous result and can be useful in practice.

2.2.2 Coherent States

Our homework will look at coherent states which are minimum uncertainty states defined as eigenstates of the annihilation operator

$$a\,|\lambda\rangle = \lambda\,|\lambda\rangle\,, \tag{2.47}$$

which implies that

$$\left\langle x^2\right\rangle_\lambda \left\langle p^2\right\rangle_\lambda = \frac{\hbar^2}{4} \tag{2.48}$$

Since we have already found $a(t)$, we know that

$$\lambda(t) = \lambda(0)e^{-i\omega t}. \tag{2.49}$$

Note that a is not Hermitian and so λ is complex in general. There is a formula for applying a position and transition operator.

$$e^{i\alpha p}e^{i\beta x}|0\rangle = |\psi\rangle. \tag{2.50}$$

So this implies that

$$\begin{aligned}
a|\psi\rangle &= ae^{i\alpha p}e^{i\beta x}|0\rangle \\
&= e^{i\alpha p}\left(e^{-i\alpha p}ae^{i\alpha p}\right)e^{i\beta x}|0\rangle \\
&= e^{i\alpha p}\left(a + ()\alpha\right)\right)e^{i\beta x}|0\rangle \\
&= ()\alpha + ()\beta|\psi\rangle,
\end{aligned} \tag{2.51}$$

where () signifies some number which we will calculate for homework.

3 Schrodinger Wave Equation

3.1 Particle in a Potential

The hamiltonian for a particle in a potential is given as

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}). \tag{3.1}$$

Our Shrodinger equation is given as

$$i\hbar\partial_t|\alpha t_0; t\rangle = H|\alpha t_0; t\rangle \tag{3.2}$$

If we want to look at it as a function of x, we have that

$$i\hbar\partial_t\langle x'|\alpha t_0; t\rangle = \langle x'|H|\alpha t_0; t\rangle, \tag{3.3}$$

and define $\psi_{\alpha t_0}(x,t) = \langle x'|\alpha t_0; t\rangle$. So this gives us that

$$\begin{aligned}
i\hbar\partial_t\langle x'|\alpha t_0; t\rangle &= \langle x'|H|\alpha t_0; t\rangle \\
&= \left\langle x'\left|\frac{\hat{p}^2}{2m} + V(\hat{x})\right|\alpha t_0; t\right\rangle \\
&= \left\langle x'\left|\frac{\hat{p}^2}{2m}\right|\alpha t_0; t\right\rangle + V(x')\psi_{\alpha t_0}(x,t) \\
&= \int\frac{1}{2m}\langle x'|\hat{p}(|x''\rangle\langle x''|)\hat{p}|\alpha t_0; t\rangle\, dx'' + V(x')\psi_{\alpha t_0}(x,t) \\
&= \frac{1}{2m}\int dx'(-i\hbar\partial_{x'}\delta(x'-x''))(-i\hbar\partial_{x''}\psi_\alpha(x'',t) + V(x')\psi_\alpha(x',t).
\end{aligned} \tag{3.4}$$

We can evaluate this as

$$-\frac{\hbar^2}{2m}\left(\partial_{x'}\partial_{x''}\psi_\alpha(x''t)\Big|_{x''=x'}\right) + V(x')\psi_\alpha(x',t). \tag{3.5}$$

This gives us the time dependant Schrodinger wave equation

$$i\hbar\partial_t\psi_\alpha(x',t) = \frac{-\hbar^2}{2m}\partial^2_{x'}\psi_\alpha(x',t) + V(x')\psi_\alpha(x',t). \tag{3.6}$$

Usually, we solve the time independent equation which we can solve as

$$\psi_\alpha(x',t) = \psi_\alpha(x')e^{-iE_\alpha t/\hbar}, \tag{3.7}$$

which comes from eigenstates only evolving in time by phase change. This leads to the time independant equation as

$$E_\alpha\psi_\alpha = -\frac{\hbar^2}{2m}\partial^2_{x'}\psi_\alpha(x') + V(x')\psi_\alpha(x'), \tag{3.8}$$

since the time dependence drops out with the substitution of the guess of solution.

3.2 Interperetation

We have the wave equation

$$i\partial_t\psi = -\nabla^2\psi\left(\frac{\hbar^2}{2m}\right) + V(x,t)\psi \tag{3.9}$$

where $\psi = \psi(x,t)$. If we think of the density

$$\rho(x,t) = |\psi(x,t)|^2 \tag{3.10}$$

we can think of a current density

$$\begin{aligned}\vec{J}(x,t) &= \frac{\hbar}{m}Im(\psi^*\vec{\nabla}\psi) \\ &= \frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^2\right)\end{aligned} \tag{3.11}$$

which leads to a continuity equation

$$\partial - t\rho + \vec{\nabla}\cdot\vec{J}(x,t) = 0 \tag{3.12}$$

which we can show with some algebra by taking the wavefunction and its complex conjugate and substituting it in. However, Born said that this cannot be the case because the continuity equation cannot allow wavefunction collapse since there would need to be an extremely large current density. This would cost a lot of energy and is completely unphysical. So we say that $\rho(x,t)$ is really the probability density and $\vec{J}$ is really a sort of probability current density.

3.2.1 Connection to Hamilton's Equations

We can write

$$\psi(x,t) = \sqrt{\rho(x,t)}\exp\left[\frac{i}{\hbar}S(x,t)\right], \tag{3.13}$$

where S has units of action. This also implie that

$$\vec{J}(x,t) = \rho\frac{\nabla S}{m} = \rho 1\text{``}v\text{''}, \tag{3.14}$$

which implies if S is action this is consistent with the Hamilton-Jacobi equation. If we substitute equation (3.13) into the original Shrodinger equation, (3.9), we get

$$i\hbar\left(\delta_t\sqrt{\rho}+\frac{i}{\hbar}\sqrt{\rho}\frac{\partial S}{\partial t}\right)=-\frac{\hbar^2}{2m}\left[\nabla^2\sqrt{\rho}+\left(\frac{2i}{\hbar}\right)(\nabla\rho)\cdot(\nabla S)-\left(\frac{1}{\hbar^2}\right)\sqrt{\rho}|\nabla S|^2+\frac{i}{\hbar}\sqrt{\rho}\nabla^2 S\right]+\sqrt{\rho}V \tag{3.15}$$

Which leads to the following equation

$$-\frac{\partial S}{\partial t}=\frac{1}{2m}|\nabla S|^2+V(x)-i\hbar\frac{\partial_t\sqrt{\rho}}{\sqrt{\rho}}-\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}+i\hbar\nabla^2 S+\frac{2i}{\hbar\sqrt{\rho}}\nabla(\sqrt{\rho})\cdot\nabla S \tag{3.16}$$

We can do some further simplification to get

$$-\frac{\partial S}{\partial t}=\frac{1}{2m}|\nabla S|^2+V(x)+V_Q(X), \tag{3.17}$$

where $V_Q(x)$ is referred to as the quantum potential defined as

$$V_Q(x)=-\frac{\hbar}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} \tag{3.18}$$

If we take the limit as $\hbar\to 0$, we get the Hamilton-Jacobi equation.

3.2.2 Particle-Wave Duality Revisited

We know that Newton said that light was particles which works really well to explain refraction. On the other hand, Young thought light was waves which explains interference very well. So to somewhat solve this, we have the Huygens-Fresnel principle which says that each point on the wave is a new source of a wave packet.

This lead to Fermat's principle which says that if you define the phase of the wave front and a related function $S(x,t)$, you can approximate the wave as traveling in the direction in which this action is minimized. In other words

$$\delta\int dS=0 \tag{3.19}$$

on the correct path. This is related to Semi-Classical approximations of quantum mechanics. This is a way to develop the theory in a classical sense and then apply leading order corrections in $\hbar$.

4 Example Problems

4.1 3D Particle in a Periodic Box

We will now solve the three dimensional particle in a box.

4.1.1 Period Boundary Conditions

We have the Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z)=E\psi(x,y,z), \tag{4.1}$$

where we have set $V(x,y,z)=0$ and imposed periodic boundary conditions

$$\psi(x+L,y,z)=\psi(x,y,z), \tag{4.2}$$

and analogously for y and z with the same L. These wavefunctions are separable in the sense that

$$\psi(x,y,z)=U_x(x)U_y(y)U_z(z), \tag{4.3}$$

which we just guessed in this case. We could also make an argument based on translational invariance which would tell us there is conserved momentum in each direction. By pluggin this in we get

$$-\frac{\hbar^2}{2m}\left(\frac{\partial_x^2 U_x}{u_x}+\frac{\partial_y^2 U_y}{U_y}+\frac{\partial_z^2 U_z}{U_z}\right)=E, \tag{4.4}$$

where we have skiped a few algebraic step. Since E is a constant, we know that

$$-\frac{\hbar^2}{2m}\frac{\partial_j^2 U_j}{U_j}=\frac{\hbar^2}{2m}k_j^2 \tag{4.5}$$

for $j=x,y,z$ So this means we can reduce this to three separate one dimensional cases and solve the equation

$$-\frac{\hbar^2}{2m}\partial_j^2 U_j(j)=\left(\frac{\hbar^2 k_j^2}{2m}\right)U_j(j). \tag{4.6}$$

We can sovle this as

$$U_j(j)=A_i e^{ik_j x}. \tag{4.7}$$

So our complete solution is

$$\psi(x,y,z)=A_x A_y A_z e^{ik_x x}e^{ik_y y}e^{ik_z z}, \tag{4.8}$$

and if we plug in our bondary conditions, we can get that

$$\psi(x+L,y,z)=e^{ik_x L}\psi(x,y,z), \tag{4.9}$$

which implies that

$$k_j L=2\pi n_j, \tag{4.10}$$

for $j=x,y,z$. So we have found our eigenvalues as

$$\frac{\hbar^2}{2mL^2}(2\pi^2)(n_x^2+n_y^2+n_z^2), \tag{4.11}$$

and

$$\psi(x,y,z)=\frac{1}{L^{3/2}}e^{i(k_x x+k_y y+k_z z)}. \tag{4.12}$$

We can write this as

$$U_E((\vec{x})=\frac{1}{L^{3/2}}e^{i\vec{k}\cdot\vec{x}} \tag{4.13}$$

where

$$\vec{k}=\left(\frac{2\pi n_x}{L},\frac{2\pi n_y}{L},\frac{2\pi n_z}{L}\right). \tag{4.14}$$

4.1.2 Real Box

If we had a real box where $x \in [0, L]$ the solution would be

$$U_E(x,y,z) = \frac{1}{L^{3/2}} \sin(k_x x) \sin(k_y y) \sin(k_z z) \tag{4.15}$$

where $k_j L = n_j \pi$ for $j = x, y, z$.

4.1.3 Free Space

Let $L \to \infty$, now we have that

$$\psi_E(\vec{x},t) = U_E(\vec{x}) e^{-iEt/\hbar} = \frac{1}{L^{3/2}} \exp\left[\frac{i(\vec{p}\cdot\vec{x} - Et)}{\hbar}\right], \tag{4.16}$$

so there is a slight difference in normalization factor based on the calculation method, but this is okay. Now we will calculate density

$$\rho(\vec{x},t) = |\psi(\vec{x},t)|^2 = \frac{1}{L^3}, \tag{4.17}$$

which is what we would expect. We can also calculate probability current density

$$\begin{aligned} \vec{J}(\vec{x},t) &= \frac{\hbar}{m} Im(\psi^* \vec{\nabla}\psi) \\ &= \frac{\vec{p}}{mL^2} \\ &= \left(\frac{\vec{p}}{m}\right)\rho. \end{aligned} \tag{4.18}$$

4.2 Particle in Finite Box

We will now talk about something extremely useful for the qualifying exam. We start with particle in a box with size l. We can write

$$\psi(\vec{x}, t=0) = \frac{1}{l^{3/2}} \sin\left(\frac{\pi x}{l}\right) \sin\left(\frac{\pi y}{l}\right) \sin\left(\frac{\pi z}{l}\right) \tag{4.19}$$

Now we release the constraints and we want to find the average energy. So we want

$$\langle H \rangle = \langle \psi(\vec{x}, t=0) | H | \psi(\vec{x}, t=0) \rangle \tag{4.20}$$

So we can introduce a complete set of energy eigenstates as

$$\langle H \rangle = \sum_{n_x, n_y, n_z} E(n_x, n_y, n_z) \langle \psi | \vec{n} \rangle \langle \vec{n} | \psi \rangle, \tag{4.21}$$

where $|\vec{n}\rangle = |n_x, n_y, n_z\rangle$ and

$$\langle \vec{x} | \vec{n} \rangle = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{x}}, \tag{4.22}$$

where $\vec{k} = \frac{2\pi}{L}\vec{n}$ and $E(\vec{n}) = \frac{\hbar^2}{2m}k^2$. So we want to take the limit as $L \to \infty$ as

$$\langle H \rangle = \int d\epsilon\, \epsilon \sum_{n_x, n_y, n_z} \delta(E(\vec{n}) - \epsilon) |\langle \psi | \vec{n} \rangle|^2. \tag{4.23}$$

So we let $f(E(\vec{n})) = |\langle \psi | \vec{n} \rangle|^2$ and we can rewrite

$$\langle H \rangle = \int d\epsilon\, \epsilon f(\epsilon) \sum_{n_x, n_y, n_z} \delta(E(\vec{n}) - \epsilon). \tag{4.24}$$

Note we have assumed that f can only depend on ϵ. This is not necessarily a good approximation for this problem, which can be seen by computing $\langle \vec{n} | \psi \rangle$. However, it is important to know this technique. So now we can use the density of state which is

$$\rho(\epsilon) = \sum_{n_x, n_y, n_z} \delta(E(\vec{n}) - \epsilon). \tag{4.25}$$

So we can do another trick and define

$$N(\epsilon) = \int_{-\infty}^{\epsilon} d\epsilon'\, \rho(\epsilon') = \sum_{n_x, n_y, n_z} \Theta(E(\vec{n}) - \epsilon) \tag{4.26}$$

So we want to figure out what $N(\epsilon)$ means. It is a cumulative function which tells the amount of states with energy less than ϵ. We can see that

$$N(\epsilon) = \frac{4\pi}{3} \left(\frac{2m\epsilon}{\hbar^2} \right)^{3/2} \frac{1}{\left(\frac{2\pi}{L}\right)^3}, \tag{4.27}$$

which implies that

$$\frac{dN}{d\epsilon} = \frac{m^{3/2}\epsilon^{1/2}L^3}{\sqrt{2}\pi^2\hbar^3}. \tag{4.28}$$

So now we have that

$$\langle H \rangle = \int d\epsilon\, \epsilon f(\epsilon) \rho \epsilon = \int d\epsilon\, \frac{1}{L^3} g(\epsilon)\rho(\epsilon), \tag{4.29}$$

where $g(\epsilon) = L^3 f(\epsilon)$.

4.3 Linear Potential

We will now solve the problem of the Linear Potential. The potential for the particle is given figure 1. So we have the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\partial_x^2 + k|x| \tag{4.30}$$

We can use some symmetries since we know that there is a symmetry over the y axis. This is because reflection commutes with the Hamiltonian. So we can just solve for $x > 0$.

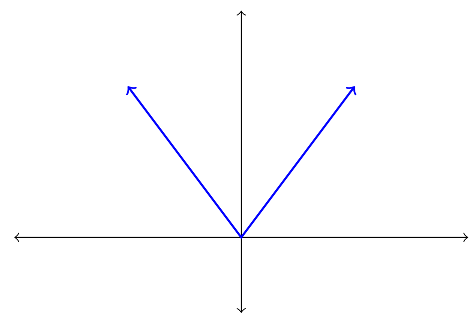

Figure 1: $V(x)$ for Linear Potential

4.3.1 Brief Introduction to Symmetry

A symmetry is an operator A which commutes with the Hamiltonian.

$$[A, H] = 0. \tag{4.31}$$

This implies there are simultaneous eigenstates. In our current case of the linear potential, if we define a specific rotation operator

$$R\,|x\rangle = |-x\rangle \tag{4.32}$$

So we know that $[R, H] = 0$. This implies that

$$\begin{aligned} R\,|\psi\rangle &= \lambda\,|\psi\rangle \\ R^2 = 1 \implies \lambda &= \pm 1 \\ \implies \langle x|R|\psi\rangle &= \langle -x|\psi\rangle \\ &= \psi(-x) \\ &= \lambda\,\langle x|\psi\rangle \\ &= \pm\psi(x). \end{aligned} \tag{4.33}$$

We can use this symmetry to get the following two Schrodinger Equations

$$\begin{aligned} \left[-\frac{\hbar^2}{2m}\partial_x^2 + k|x|\right]\psi(x) &= E\psi(x) \\ \left[-\frac{\hbar^2}{2m}\partial_x^2 + k|x|\right]\psi(-x) &= E\psi(-x) \end{aligned} \tag{4.34}$$

which implies that

$$\psi(x) = e^{i\phi}\psi(-x) = e^{2i\phi}\psi(x) \tag{4.35}$$

where $\phi = 0 \ldots \pi$. this implies that $\psi(x) = \pm\psi(-x)$. We can also think of complex conjugation and get

$$\left[-\frac{\hbar^2}{2m}\partial_x^2 + k|x|\right](\psi(x) + \psi^*(x)) = E(\psi(x) + \psi^*(x)). \tag{4.36}$$

this implies that I can find a real eigenstate if it is non-degenerate. Even if it is degenerate, you can find a complete set of them. Can always multiply by a phase. THIS MAY HELP on midterm.

4.3.2 Solution to Linear Potential

Because of the symmetries, we can just solve for $x > 0$ and then construct the rest of the solution by symmetry. So we are solving the equation

$$\left[\frac{\hbar^2}{2m}\partial_x^2 + kx\right]\psi(x) = E\psi(x). \tag{4.37}$$

Need to remember that once solution is found for $x > 0$, only solutions satisfying $\psi(x) = \pm\psi(-x)$ will be allowed. This mean in particular that for minus sign $\psi(0) = 0$ and for plus sign $\psi'(0) = 0$. When I speak of $\pm$ I mean $\pm$ in the sense $\psi(x) = \pm\psi(-x)$.
So if we let $x = yx_0$ and then $p = \frac{p'}{y}$. So we know have that

$$\left[-\frac{\hbar^2}{2mx_0^2}\partial_y^2 + (kx_0)y\right]\psi = E\psi \tag{4.38}$$

If we let

$$kx_0 = \frac{1}{2mx_0^2} \implies x_0 = \left(\frac{1}{2m\hbar}\right)^{1/3} \tag{4.39}$$

which implies that

$$\left[-\hbar^2\partial_y^2 + y\right]\psi = \left(\frac{E}{k\left(\frac{1}{2m\hbar}\right)^{1/3}}\right)\psi \tag{4.40}$$

Note that this is effectively making $m = 1/2$ and $k = 1$. We will call $\mathbb{E} = \frac{E}{k\left(\frac{1}{2m\hbar}\right)^{1/3}}$. So we can shift $y \to y + \mathbb{E}$ and then we have that

$$[-\hbar^2\partial_y^2 + y]\psi = \psi. \tag{4.41}$$

This is really only because we have a linear potential. If $\hbar = 1$, then this is the Airy equation whose solutions are called Airy functions. To solve this,we will go to p space which leads to the following equation

$$(p^2 + i\hbar\partial_p)\psi = 0. \tag{4.42}$$

So we know that

$$\frac{d\psi}{dp} = \frac{i}{\hbar}p^2\psi \implies \psi(p) = \psi(0)e^{-ip^3/3\hbar} \tag{4.43}$$

So we have the solution in momentum space. So we can say that

$$\begin{aligned}
\psi(x) &= \langle x|\psi\rangle \\
&= \int dp\,\langle x|p\rangle\,\langle p|\psi\rangle \\
&= \int dp\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\psi(p) \\
&= \psi(0)\int_{-\infty}^{\infty}\frac{dp}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}(pxi - p^3/3)}
\end{aligned} \tag{4.44}$$

We can solve this using asymptotic evaluation of integrals. We take limit as $\hbar \to 0$, which is some sort of semi-classical approximation, we can get an approximate solution for this integral by using Laplace's method which comes out to be (note we switched from y to x.

$$\psi(x) = \psi(0)e^{i\pi/4}\left(\frac{1}{\sqrt{-2\sqrt{x}}}\exp\left[\frac{2x^{3/2}}{3\hbar}\right] + \frac{1}{\sqrt{2\sqrt{x}}}\exp\left[\frac{-i2x^{3/2}}{3\hbar}\right]\right) \tag{4.45}$$

There is a sign error here and really $x \to -x$ which was lost during the Fourier transform. This allows us to get the relative phase between the two. So our final answer is really given by a solution to airy equation

$$\psi(x) = \frac{i\psi(0)}{\sqrt{2\sqrt{-x}}}e^{i\pi/4}\left(e^{i\frac{2}{3\hbar}(-x)^{3/2}} - ie^{-\frac{i2}{3\hbar}(-x)^{3/2}}\right) \tag{4.46}$$

which agrees with our asymptotic evaluation.

5 WKB Approximation

This is a technique to reduce quantum problem to classical problem. The way to do that is to take $\hbar \to 0$ in a specific way. We can't ignore $\hbar$, we need to find lowest order corrections in terms of $\hbar$. The outcome is that to lowest order we will just have quantization of energy levels. We start again with the Schrodinger equation which satisfies

$$-\frac{\hbar^2}{2m}\frac{d^2u_E}{dx^2} + V(x)u_E(x) = Eu_E(x) \tag{5.1}$$

which we can write as

$$\frac{d^2u_E}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))u_E(x) = 0 \tag{5.2}$$

5.1 Motivation

Our motivation is that if we have $e^{ipx/\hbar}$ then as $\hbar \to 0$, we have that $k = p/\hbar \to \infty$, so it is rapidly oscillating. So we want to say that

$$u_E(x) \sim \exp\left[ikx\right], \tag{5.3}$$

if $V(x)$ is slow. In a classical system, we have that $\frac{\hbar^2k^2][2m}{=}E - V(x)$ which implies that

$$k = \pm\sqrt{\frac{2m}{\hbar^2}(E - V(x)}. \tag{5.4}$$

5.2 Formal Derivation

Motivated by previous section we are going to define $k(x)$ in the same mathematical form as before, although it is **not** necessarily a wavevector anymore. We now have

$$u_E(x) = \exp\left[\frac{i}{\hbar}w(x)\right], \tag{5.5}$$

where $w(x)$ is some complex function. We now plug into the Schrodinger equation to get that

$$i\hbar\frac{d^2w}{dx^2} - \left(\frac{dw}{dx}\right)^2 + \hbar^2 \underbrace{\left(\frac{2m}{\hbar^2}(E - V(x)\right)}_{k(x)^2} = 0 \tag{5.6}$$

If $k(x)$ is slowly varying, then we expect $w(x)$ to be slowly varying and so

$$\left|\frac{\hbar d^2w}{dx^2}\right| \ll \left(\frac{dw}{dx}\right)^2, \tag{5.7}$$

which leads us to ignore the second derivative. We can now solve the equation iteratively and we have to first order

$$\begin{aligned}
\frac{dw}{dx} &= \sqrt{\hbar^2 k(x)^2 + i\hbar\frac{d^2w}{dx^2}} \\
\implies \frac{dw_0}{dx} &= \pm\hbar k(x) \\
\implies \frac{dw_1}{dx} &= \pm\sqrt{\hbar^2 k(x)^2 + i\hbar\frac{d^2w_0}{dx^2}} \\
&\vdots
\end{aligned} \tag{5.8}$$

where we can solve for arbitrarily many terms in the series. So we have that

$$w_0(x) = \pm\hbar\int_{-\infty}^{x} dx'\, k(x') \tag{5.9}$$

which implies that

$$u_E(x) = \exp\left[\frac{i}{\hbar}w_0(x)\right] = \exp\left[\pm i\int_{-\infty}^{x} dx'\, k(x')\right]. \tag{5.10}$$

We can calculate a current operator for this as

$$\begin{aligned}
\vec{J} &= (u^*\nabla u - u\nabla u^*)\frac{i\hbar}{2m} \\
&= \frac{\nabla S}{m},
\end{aligned} \tag{5.11}$$

where $u = \sqrt{\rho}e^{is}$. However, we need that

$$\partial_t \rho + \nabla\cdot\vec{J} = 0, \tag{5.12}$$

which is an issue since $\nabla\cdot\vec{J} \neq 0$ and therefore the continuity equation would not be satisfied. However, we will fix this with the second order term in the series. For the second order,

$$\frac{dw_1}{dx} = \pm\sqrt{\hbar^2 k(x)^2 \pm i\hbar^2 k'(x)}. \tag{5.13}$$

We want to know the conditions for the proper "slowness" of variation for this approximation to work. We know that $|k'(x)| \ll k(x)^2$ which implies that

$$\frac{|V'(x)|}{\sqrt{E - V(x)}}\sqrt{\frac{2m}{\hbar^2}} \ll \frac{2m}{\hbar^2}(E - V(x)) \implies |V'(x)| \ll \sqrt{\frac{2m}{\hbar^2}}(E - V(x))^{3/2}, \tag{5.14}$$

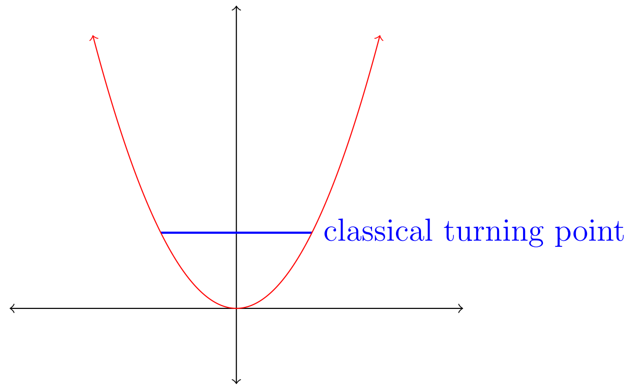

Figure 2: Bound state of WKB approximation, classical sense

for the approximation to hold. We can do an expansion to get that

$$\frac{dw_1}{dx} = \pm\hbar k(x)\left(1 \pm \frac{i}{2}\frac{k'(x)}{k(x)^2}\right) \tag{5.15}$$

which we can solve quite easily as

$$w_1(x) = w_0(x) \pm \frac{i\hbar}{2}\int \frac{dx'}{k(x')}\frac{dk}{dx'} \tag{5.16}$$

We can cancel out the partial derivative here (kind of sloppy but it works) and evaluate this integral as a logarithm and get that

$$u_E(x) = e^{iw_1(x)} = \frac{A}{\sqrt{k(x)}}e^{iw_0(x)}, \tag{5.17}$$

which is the normal form of the WKB approximation. So under certain conditions where the potential slowly varying compared to wavelength of the wavefunction, we can write this approximation as

$$\psi(x) \approx \frac{1}{\sqrt{k(x)}}e^{i\int_{-\infty}^{x} k(x')dx'} \tag{5.18}$$

where $k(x)$ is the classical wave vector given as

$$k(x) = \sqrt{\frac{2m}{\hbar^2}(E - V(x))}, \tag{5.19}$$

with the condition that $|k'(x)| \ll k(x)^2$. One way to think of this is to look at classical momentum and think of the continuity equation with current density. Then we can do an asymptotic evaluation of the integral. This will give us the wavefunction, but now we want to solve for E.

5.3 Evaluating the Eigenvalues

In our bound state, we can draw a picture as in figure 2 We know that

$$\psi_{WKB}(x) = \frac{1}{k(x)^2}\left[c_+e^{i\int_0^x dx'k(x')} + c_-e^{-i\int_0^x k(x')dx'}\right], \tag{5.20}$$

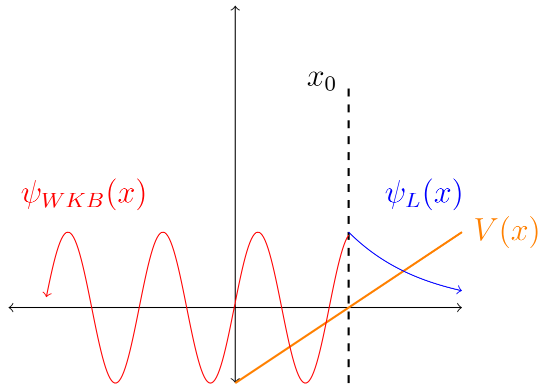

Figure 3: WKB approximation near turning point

where $k(x)$ is as defined in (5.19). If we look near the turning point, then the potential looks linear. So if look at the wavefunction here, we have a region far from the turning point where the WKB approximation will still be valid, but there is a divergence near the turning point. Since the wavefunction must be continuous going from the region where the WKB approximation holds to the bad region, we can approximate by airy function. This is shown in figure 3 So choose a point x_0 and we must match the wavefunction ψ_L and ψ_{WKB}. Here,

$$\psi_{WKB}(x_0) = \psi_L(x_0) \tag{5.21}$$

$$\psi'_{WKB}(x_0) = \psi'_L(x_0). \tag{5.22}$$

So we can find the classical turning point as

$$\psi_L(x_0) = \frac{1}{\sqrt{\pi}(x_t - x)^{1/4}} \cos\left(\frac{2}{3}\lambda(x_t - x)^{3/2} - \frac{\pi}{4}\right), \tag{5.23}$$

where

$$\lambda = \left(\frac{V'(x_t)}{\hbar^2}\right)^{3/2} \tag{5.24}$$

So we can taylor expand the cos function to get

$$\psi_L(x) = \frac{1}{2\pi^{1/2}(x_t - x)^{1/4}}\left[\exp\left(i\frac{2}{3}\lambda(x_t - x)^{3/2} - \frac{i\pi}{4}\right) + \exp\left(-i\frac{2}{3}\lambda(x_t - x)^{3/2} + \frac{i\pi}{4}\right)\right], \tag{5.25}$$

and we can also replace the energy with potential at x_t in the term for $k(x)$ and taylor expand to get

$$\begin{aligned} k(x) &= \sqrt{\frac{2m}{\hbar^2}(V(x_t) - V(x))} \\ &= \sqrt{\frac{2m}{\hbar^2}V'(x_t)}(x_t - x)^{1/2}. \end{aligned} \tag{5.26}$$

So we now just need to evaluate some integrals.

$$\begin{aligned} \int_0^x dx' k(x') &= \int_0^{x_t} dx' k(x') - \int_x^{x_t} dx' k(x') \\ &= \int_0^{x_t} dx' k(x') + \frac{2}{3}\sqrt{\frac{2m}{\hbar^2}V'(x_t)}(x_t - x)^{3/2} \end{aligned} \tag{5.27}$$

Now we notice that the second term in this expression is the same as the expression of ψ_L up to an additional constant of $-i\pi/4$. So we have that

$$\psi_L(x \sim x_0) = \zeta \psi_{WKB}(x \sim x_0) \tag{5.28}$$

Which implies that

$$c_+ \exp\left(i \int_0^{x_t} dx' k(x')\right) = \zeta e^{-i\pi/4} \tag{5.29}$$

$$c_- \exp\left(-i \int_0^{x_t} dx' k(x')\right) = \zeta e^{i\pi/4} \tag{5.30}$$

which gives us c_+, c_-. So we have that

$$c_+ \exp\left(i \int_0^{x_t} dx' k(x')\right) = c_- \exp\left(-i \int_0^{x_t} dx' k(x')\right) e^{-i\pi/2} \tag{5.31}$$

which leads to

$$c_- = e^{i\pi/2} c_+ \exp\left(\int_0^{x_t} dx' k(x') + i \int_{x_t}^0 dx'(-k(x'))\right). \tag{5.32}$$

This is saying that c_- is the phase that the particle picks up as it goes from x_0 to the classical turning point and then the phase as it goes from the turning point back to zero. There is an additional factor of $e^{i\pi/2}$ which comes from the matching of the wavefunctions in the WKB approximation. More formally this is known as part of the WKB connection formula. There is also a way in Landau-Litchitz to get this formula. We can repeat the argument at the other turning point to get

$$c_+ = e^{i\pi/2} c_- \exp\left(\text{Similiar to other case}\right) \tag{5.33}$$

So this means that the integral over the loop going from zero to the turning point on the right to the turning point on the left and back to zero, we get that

$$\oint dx' k(x') = (2n+1)\pi. \tag{5.34}$$

So if then substitute the formula for k into this integral. We find that we cannot satisfy the matching of the boundary conditions unless we have specific values of E. This is the quantization. This leads to the important WKB formula

$$\oint dx' p(x') = (2n+1)\pi\hbar. \tag{5.35}$$

Interestingly, this is the Bohr-Sommerfeld quantization condition except no +1 in the factor. For the Hydrogen atom, this doesn't matter.

5.4 WKB Example Problem

We will apply this formalism to the Quantum Harmonic oscillator. We have the Hamiltonian

$$H = \frac{p^2}{2m} + V(x), \tag{5.36}$$

where $V(x) = \dfrac{1}{2}kx^2$. The first thing we do is compute the classical momentum. This is given as

$$p(x) = \sqrt{2m(E - V(x)} = \hbar k(x), \tag{5.37}$$

where we have defined k to be this way. So we know that

$$\psi(x) = \frac{1}{\sqrt{k(x)}}\left[c_+ \exp\left(i\int_0^x k(x')dx'\right) + c_- \exp\left(-i\int_0^x k(x')dx'\right)\right]. \tag{5.38}$$

To get c_+, c_-, we can use the WKB connection formula where the turning point is where $p(x_t) = 0$ which implies that $v(x_t) = E$. It is clear by symmetry that

$$|c_+| = |c_-|. \tag{5.39}$$

So we want to find the relative phase by doing a trick and writing

$$\begin{aligned}\psi(x) = \frac{1}{\sqrt{k(x)}}\Bigg[&c_+ \exp\left(i\int_0^{x_t} k(x')dx'\right)\exp\left(-i\int_x^{x_t} k(x')dx'\right)\\ &+ c_- \exp\left(-i\int_0^{x_t} k(x')dx'\right)\exp\left(i\int_x^{x_t} k(x')dx'\right)\Bigg]\end{aligned} \tag{5.40}$$

We know that we have the relation between c_- and c_+ which is given by an explicit formula. We will leave the rest of this for homework and so we will move on to calculating the energies. We can evaluate the energy as

$$\oint dx\, p(x) = \left(n + \frac{1}{2}\right)h \tag{5.41}$$

So we have

$$\begin{aligned}\oint dx\, p(x) &= \int_0^{x_t} dx'\, p(x') + \int_{x_t}^0 dx'\,(-p(x')) + \int_0^{-x_t} dx'\,(-p(x')) + \int_{-x_t}^0 dx'\, p(x')\\ &= 2\int_0^{x_t} p(x')\, dx' + 2\int_{-x_t}^0 p(x')\, dx'\\ &= 2\int_{-x_t}^{x_t} dx'\, p(x')\\ &= 2\int_{-x_t}^{x_t} dx' \sqrt{2m\left(E - \frac{1}{2}kx^2\right)}\\ &= 2\sqrt{mk}\int_{-x_t}^{x_t} dx' \sqrt{x_t^2 - x'^2}\end{aligned} \tag{5.42}$$

and we simple need to evaluate this integral. So we make the subsitution

$$x' = x_t\cos\theta \tag{5.43}$$

and so we can evaluate the integral as

$$2\sqrt{mk}x_t^2\int_\pi^0 d\theta(-\sin\theta)\sin(\theta) = 2\frac{\pi}{2}x_t^2\sqrt{mk} \tag{5.44}$$

We now substitute in E to get the final answer of

$$2\pi E\sqrt{\frac{m}{k}} \tag{5.45}$$

So we get that

$$2\pi E_n\sqrt{\frac{m}{k}} = \left(n+\frac{1}{2}\right)h \implies E_n = \hbar\omega\left(n+\frac{1}{2}\right), \tag{5.46}$$

where $\omega = \sqrt{\frac{k}{m}}$. Usually it does not work out exactly, but here it does. Usually this approximation is bad at small n, but is much better at larger n, (≈ 10).

6 Propagators

This is a concept which leads towards a Feynman path integral. This path integral is useful for relativity and a good way of visualizing quantum mechanics. So say you want to calculate $\psi(x,t)$, given $\psi(x',t_0)$, some earlier time. We know that

$$\begin{aligned}\psi(x,t) &= \langle x,|\psi(t)\rangle \\ &= \left\langle x|e^{-iH(t-t_0)/\hbar|\psi(t_0)}\right\rangle \\ &= \int dx' \underbrace{\left\langle x|e^{-iH(t-t_0)/\hbar}|x'\right\rangle}_{K(x,t,x't_0)\to propagator} \underbrace{\langle x'|\psi(t_0)\rangle}_{\psi(x',t_0)}\end{aligned} \tag{6.1}$$

We can make an analogy to classical electrostatics where $\nabla^2\phi = \rho$ implies that

$$\phi(x) = \int dx' \underbrace{\left(\frac{1}{|x-x'|}\right)}_{propagator}\rho(x') \tag{6.2}$$

where we can check this satisfied the equation since

$$\nabla^2\frac{1}{|x-x'|} \tag{6.3}$$

which implies that if we do the integral, this is self consistent. We can also show that the quantum propagator K solves the Schrodinger equation. Some properties are

$$K(xt_0;x't_0) = \delta(x-x') \tag{6.4}$$

$$K(xt;x't_0) = 0 \quad t<t_0 = \delta(x-x')\Phi(t-t_0) \tag{6.5}$$

6.1 Free Particle Propagator

We want to calculate

$$K = \left\langle x|e^{-ip^2(t-t_0)/2m\hbar}|x'\right\rangle. \tag{6.6}$$

After inserting a complete set of states and doing some calculates we recover

$$\sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\exp\left(\frac{im(x-x')^2}{2\hbar(t-t_0)}\right) \tag{6.7}$$

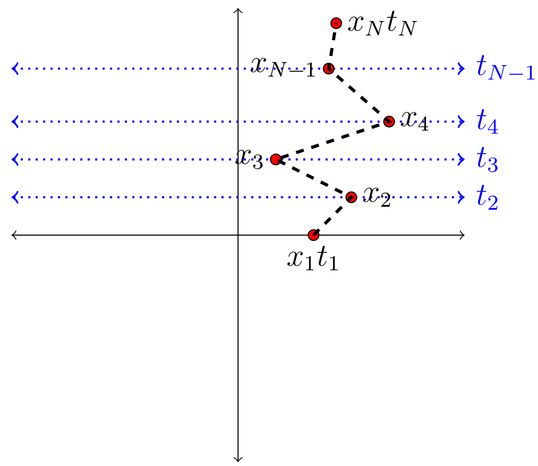

Figure 4: Path Integral. Only one possible path is shown.

7 Path Integrals

We want to reforumlate quantum mechanics in a new way. So our basic object is

$$|xt\rangle_H\,, \tag{7.1}$$

a particle at x at time t and we want to calculate

$$K = \langle xt|x't'\rangle\,, \tag{7.2}$$

which is the probability of a particle going from $x't'$ to xt. First we notice that these are eigenstates of a Hermitian operator and form a complete set of states, so we have that

$$\int dx' \; |x't\rangle \langle x't| = 1, \tag{7.3}$$

so we can write

$$\langle xt|x't'\rangle = \int dx'' \; \langle xt|x''t''\rangle \langle x''|x't'\rangle \tag{7.4}$$

So we can continue to break it up into multiple slices. Switching notation, what we want to calculate is

$$\langle x_N t_N|x_1 t_1\rangle \tag{7.5}$$

where $t_N > t_1$. So we can break it up into a series of

$$t_N > t_{N-1} > \ldots t_2 > t_1, \tag{7.6}$$

and then propogate

$$\int dx_2 dx_3 \ldots d_{x_{N-1}} \langle x_N t_N|x_{N-1} t_{N_1}\rangle \ldots \langle x_3 t_3|x_2 t_2\rangle \langle x_2 t_2|x_1 t_1\rangle\,. \tag{7.7}$$

So we have essentially broken time up into segments and then propagated. This is shown in figure 4 Feynhman drew inspiration from Dirac to say that

$$\langle Xt|x't'\rangle \sim \exp\left(i\frac{S(xt;x't')}{\hbar}\right) \tag{7.8}$$

where S is the action defined as

$$S(xt't') = \int_{x't'}^{xt} L(x_1,t_1)\,dt_1, \tag{7.9}$$

except that this action depends on the path. However, if you are going through two points close together in some sense, then we can say that the line is probably classically linear. So we have that if $|t_2 - t - 1|$ small in some sense, then

$$\langle x_2t_2|x_1t_1\rangle \propto \exp\left(\frac{i}{\hbar}S(1,2)\right). \tag{7.10}$$

This implies that

$$\langle x_Nt_N|x_1t_1\rangle \propto \int dx_{N-1}\dots dx_2\,\exp\left(\frac{i}{\hbar}S(N,N-1)\right)\dots\exp\left(\frac{i}{\hbar}S(3,2)\right)\exp\left(\frac{i}{\hbar}S(2,1)\right), \tag{7.11}$$

which we can write as

$$\int \exp\left(\frac{i}{\hbar}\sum_{j=1}^{N-1} S(j+1,j)\right). \tag{7.12}$$

We this sum as

$$\begin{aligned}\sum_{j=1}^{N-1} S(j+1,j) &= \int_{x_1,t_1}^{x_2,t_2} L + \int_{x_2t_2}^{x_3t_3} L \dots + \int_{x_{N-1}}^{N} L \\ &= \int_{x_1t_1}^{x_Nt_N} dt' L(x'(t'),x'(t'),t') \\ &= S_Q(x_Nt_N, x_{N-1}t_{N-1},\dots,x_1t_1),\end{aligned} \tag{7.13}$$

where the Q is to separate the quantum action from the classical action. This implies that

$$\langle x_Nt_N|x_1t_1\rangle \propto \int \exp\left(\frac{i}{\hbar}S_Q(x_1t_1,\dots,x_Nt_N)\right)dx-1\dots dx_{N-1}. \tag{7.14}$$

7.1 Finding Proptionality Constant

We now want to find the proportionality constant in this equation. We know that

$$\langle x_2t_2|x_1t_1\rangle = \frac{1}{W(\Delta t)}\exp\left(\frac{i}{\hbar}S(x_2t_2,x_1t_1)\right) \tag{7.15}$$

Since the proportionality constant W should be independent of the potential, we can set $V=0$ and write the action as

$$S(x_2t_2,x_1t_1) = \int_{t_1}^{t_2} dt'\left(\frac{m}{2}\dot{x}^2\right), \tag{7.16}$$

where we assume that in short time periods the particle acts by moving on a classical trajecotyr which implies that

$$x(t') = x_1 + \left(\frac{x_2 - x_1}{t_2 - t_1}\right)(t' - t_1), \tag{7.17}$$

which implies that

$$S = \frac{m}{2}\frac{(x_2 - x_1)^2}{t_2 - t_1}, \tag{7.18}$$

which we can substitute into our equation to get that

$$\langle x_2 t_2 | x_1 t_1 \rangle = \frac{1}{W(\Delta t)} \exp\left(\frac{im}{2\hbar}\frac{(x_2 - x_1)^2}{\Delta t}\right). \tag{7.19}$$

Since we know that $\langle xt | x't \rangle = \delta(x - x')$, as $\Delta t \to 0$, we need

$$\langle x_2 t_2 | x_1 t_1 \rangle \to \delta(x_2 - x_1). \tag{7.20}$$

In order for this to be true, we can normalize the equation as

$$\int_{-\infty}^{\infty} dx_2 \frac{1}{W(\Delta t)} \exp\left(\frac{im}{2\hbar}\frac{(x_2 - x_1)^2}{\Delta t}\right) = 1, \tag{7.21}$$

where if we do the Gaussian integration, we can find that

$$W(\Delta t) = \sqrt{\frac{2\pi i \hbar \Delta t}{m}} \tag{7.22}$$

which gives us that

$$\langle x_2 t_2 | x_1 t_1 \rangle = \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \exp\left(\frac{i}{\hbar} S(x_2 t_2, t_1 t_1)\right), \tag{7.23}$$

and so in the general case, we get

$$\langle x_N t_N | x_1 t_1 \rangle = \int dx_2 \dots dx_{N-1} \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{N/2-1} \exp\left(\frac{i}{\hbar}\int_{\gamma : t_1}^{t_n} L(x'(t'), t')\right), \tag{7.24}$$

which is the Feynman path integral. γ is some path over which we integrate the Lagrangian. We often see this written as

$$\int_{x, t_1}^{x_N, t_N} Dx e^{\frac{i}{\hbar} S[x(t)]} \tag{7.25}$$

7.2 Relation to other Formulations

7.2.1 Classical Limit

We want to recover the classical formulation from this quantum formulation. So in the limit as $\hbar \to 0$, we can use stationary phase method to calculate this integral. Intuitively, this means we only get contributions around the point

$$\frac{\delta}{\delta x_p} S\left[x_1 t_1, \dots, x_N t_N\right], \tag{7.26}$$

which is the principle of least action from classical mechanics and so the classical path is dominant. This is very useful in practice.

7.2.2 Connection to Schrodinger Equation

The details to prove this is very algebraically involved and we will not do a complete writeup here (its in Sakurai), but we will give an outline. We want to show that

$$-i\hbar\partial_{t_N}\psi(x_Nt_N) = -\frac{\hbar^2}{2m}\nabla^2\psi(x_Nt_N) + V(x_Nt_N)\psi(x_Nt_N). \tag{7.27}$$

It can be shown that it is sufficient to check that this is true if we the wavefunction equal to the propagator

$$\psi(x_Nt_N) = \langle x_Nt_N|x_1t_1\rangle . \tag{7.28}$$

We don't really want to deal with full path integral, so we want to break up the integral into its parts and focus on expressions like

$$\langle x_Nt_N|x_1t_1\rangle = \int sx_{N-1} \langle x_Nt_N|x_{N-1}t_{N-1}\rangle \langle x_{N_1}t_{N-1}|x_1t_1\rangle , \tag{7.29}$$

where we observe that $|t_N - t_{N_1}| = \Delta t$ is small. We can get an expression to substitute into the Schrodinger equation which should work out. So we can show that these approaches are completely consistent with each other.

8 Quantum Particle in an Electromagnetic Field

We will start with talking about regular electrostatic potentials which will be a prelude to vector potentials. The real point is to talk about gauge invariance. So we have our normal free particle Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(x), \tag{8.1}$$

and we want to look at the effect of

$$V(x) \to V(x) + \phi(t) \tag{8.2}$$

on the solution. So we want to find the solution to the Schrodinger equation with the extra phase dependence. So we can write

$$\left[-\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - v(x) - \phi(t)\right]\psi' = 0. \tag{8.3}$$

Classically this would be easy since shifting the potential by a constant factor would not change the solution. So we know that $\psi'(x,t)$ is almost equal to $\psi(x,t)$. So we guess

$$\psi'(x,t) = \psi(x,t)e^{i\Lambda(t)}, \tag{8.4}$$

then we get that $N(t) = \frac{1}{\hbar}\int_{-\infty}^{\infty}\phi(t')\,dt'$, which implies that

$$\left(\frac{1}{\hbar}\partial_t\Lambda - \phi(t)\right)\psi = 0 \implies \psi'(x,t) = \psi(x,t)\exp\left(\frac{i}{\hbar}\int_{-\infty}^{\infty}\phi(t')\,dt'\right). \tag{8.5}$$

We know that changing the phase doesn't do that much to the physical meaning of the wave-funciton, but it can lead to interference, however potential gradients matter much more. Potential gradients can have non-local effects. If we think of the two slit experiments, we will have a new one where we split a beam and each beam passes through two metallic tubes connected by a battery and then the beams are brought back together. So we can write the equation

$$\left[-\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - V(x) - \phi_j(t)\right]\psi_j(x,t) = 0. \tag{8.6}$$

We can choose

$$\phi_1(t) = \frac{\phi_0}{2}\ ; \phi_2(t) = \frac{-\phi_0}{2}. \tag{8.7}$$

Note that ϕ_0 comes from the battery. There is no electric field where the particle is in tube but there is one outside. So we can write

$$\psi(x,t)_j = \psi_0(x,t)\exp\left(\frac{i}{\hbar}\int_0^\infty \phi(t')_j\, dt'\right), \tag{8.8}$$

where $\phi_0(x,t)$ is the $\phi_0 = 0$ solution. So we can solve for both wavefunctions as

$$\psi_1(x,t) = \psi_0(x,t)\exp\left(\frac{i(t_2-t_1)}{2\hbar}\phi_0\right) \tag{8.9}$$

$$\psi_2(x,t) = \psi_0(x,t)\exp\left(\frac{-i(t_2-t_1)}{2\hbar}\phi_0\right), \tag{8.10}$$

which implies that the general solution is given as

$$\begin{aligned}\psi(x,t) &= \psi_0(x,t)\left[\exp\left(\frac{i(t_2-t_1)}{2\hbar}\phi_0\right) + \exp\left(\frac{-i(t_2-t_1)}{2\hbar}\phi_0\right)\right] \\ &= 2\psi_0(x,t)\cos\left(\frac{t_2-t_1}{2\hbar}\phi_0\right).\end{aligned} \tag{8.11}$$

Classically the particle would not feel any affect, yet here we see quantum effects.

8.1 Vector Potential

We can get from Newton's laws the basic force law as

$$m\frac{d^2x}{dt^2} = q\left(\vec{E} + \vec{v}\times\vec{B}\right). \tag{8.12}$$

So we can define a Hamiltonian for electrostatics as

$$H = \left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + e\phi(\vec{x}), \tag{8.13}$$

where

$$\vec{B} = \vec{\nabla}\times\vec{A}\ ; \vec{E} = -\nabla\phi, \tag{8.14}$$

where ϕ and A are auxiliary fields that are not observable. We can use gauge invariance to say that if we shift $\vec{A}\to\vec{A}+\nabla\Lambda$, then $\vec{B}$ does not change. So thing for $\phi to \phi + \delta\phi$ and $\vec{E}$.
MISSED NOTES

9 Aharonov Bohm Effect

If we look at the spectrum of a particle that is trapped on a cylinder (NEED to Fill in notes), we get the final solution of

$$E(n, k_z) = \frac{\hbar^2 k_z^2}{2m} + \frac{\hbar^2}{2mR^2}\left(n - \frac{\Phi}{\Phi_Q}\right)^2 \tag{9.1}$$

where $\Phi_Q = hc/e$ is a flux quantum. This implies that even though the particle never sees the magnetic field, it still knows about it. The more traditional version of the Aharonov Bohm effect is an interference experiment where there is a source and a detector and a magnetic field in the center which the particle does not pass through. So we have that

$$P(\Phi) = |\langle x_D(t)|x_S(0)\rangle|^2, \tag{9.2}$$

the probability from going from the source to the detector. We will use path integrals here. So we have that

$$|\langle x_D(t)|x_S(0)\rangle|^2 = \int_{x(0)=x_s}^{x(t)=x_D} \mathcal{D}x \, \exp\left(\frac{i}{\hbar}S[x(\tau)]\right), \tag{9.3}$$

where the action is given as

$$S[x(\tau)] = \int dz \left[\frac{m}{2}\dot{x}^2 - V(x(z)) + \frac{e}{c}\dot{x}\bar{A}(x(\tau))\right] \tag{9.4}$$

Remark 9.1. *We need to check that the action is gauge invariant. So if we perform a gauge transformation*

$$\bar{A} \mapsto \bar{A} + \nabla\Lambda \tag{9.5}$$

the action transforms as

$$S \mapsto S + \frac{e}{c}\int dz\, \dot{x} \cdot \nabla\Lambda \tag{9.6}$$

which means that we get

$$\langle x_D(t)|x_S(0)\rangle \mapsto \langle x_D(t)|x_S(0)\rangle \exp\left[\frac{-ie}{\hbar c}\left(\Lambda(x_D(t)) - \Lambda(x_S(0))\right)\right], \tag{9.7}$$

which means the path integral formulation is gauge invariant.

Now back to the problem at hand. We have that

$$\begin{aligned} S &= \int dz\, \frac{m\dot{x}^2}{2} - V(x(\tau)) + \frac{e}{c}\int \frac{d\vec{x}}{dt} \cdot \vec{A}(x(\tau)) \\ &= S_0 + \frac{e}{c}\underbrace{\int d\tau \frac{d\vec{x}}{d\tau} \cdot \vec{A}(x(z))}_{f[x[\tau]]}, \end{aligned} \tag{9.8}$$

where the $f[x[\tau]]$ only depends on τ formally. Now we consider path independence. If we consider the two paths γ_1 and γ_2 which do not pass through the magnetic flux. We have that

$$\begin{aligned} f[\gamma_1] - f[\gamma_2] &= \int_{x_S \gamma_1}^{x_D} dx \cdot A - \int_{x_S \gamma_2} dx \cdot A \\ &= \oint_{\gamma_1 - \gamma_2} dx \cdot A(x) \\ &= \int_{\gamma_1 - \gamma_2} d\vec{a} \cdot (\nabla \times A) \\ &= \Phi_{\gamma_1 - \gamma_2}, \end{aligned} \tag{9.9}$$

which is just the flux through the enclosed area between the loops. So choose some reference point γ_0. So we have that

$$S[x(\tau)] = S_0[x(\tau)] + \frac{e}{c} f[\gamma_0] + \frac{e}{c}(f[x(\tau)] - f[\gamma_0]) \tag{9.10}$$

So we only need to consider paths below and above the magnetic cylinder. So we have that

$$S[x(\tau) \in \gamma_{\text{above}}] = S_0 + f[\gamma_0] + 0 \tag{9.11}$$

$$S[x(\tau) \in \gamma_{\text{below}}] = S_0 + f[\gamma_0] + \frac{e}{c}\Phi, \tag{9.12}$$

So we have that

$$\begin{aligned} \langle x_D(t) | x_S(0) \rangle &= \int \mathcal{D}x \exp\left(\frac{i}{\hbar} S[x(\tau)]\right) \\ &= \int_{\text{above}} \mathcal{D}x \exp\left(\frac{i}{\hbar} S[x(\tau)]\right) + \int_{\text{below}} \mathcal{D}x \exp\left(\frac{i}{\hbar} S[x(\tau)]\right) \\ &= \int_{\text{above}} \mathcal{D}x \exp\left(\frac{i}{\hbar}\left(S_0 + \frac{e}{c} f(x_0)\right)\right) + \int_{\text{below}} \mathcal{D}x \exp\left(\frac{i}{\hbar}\left(S_0 + \frac{e}{c} f(x_0)\right)\right) e^{2\pi i \Phi/\Phi_Q} \end{aligned} \tag{9.13}$$

So define

$$t_{\text{above}} = \int_{\text{above}} \mathcal{D}x \exp\left(\frac{i}{\hbar} S_0\right) \; ; \; t_{\text{below}} = \int_{\text{below}} \mathcal{D}x \exp\left(\frac{i}{\hbar} S_0\right), \tag{9.14}$$

then we have that

$$\langle x_D(t) | x_S(0) \rangle = e^{i \frac{e}{c} f(\gamma_0)} \left((t_{\text{above}} + t_{\text{below}} e^{2\pi i \Phi / |phi_Q} \right), \tag{9.15}$$

which implies that

$$\begin{aligned} P &= | \langle x_D(t) | x_S(0) \rangle |^2 \\ &= \left| t_{\text{above}} + t_{\text{below}} e^{2\pi i \Phi/\Phi_Q} \right|^2 \\ &= |t_{\text{above}}| + |t_{\text{below}}| + 2|t_{\text{above}}| \cdot |t_{\text{below}}| \cos\left(\frac{2\pi\Phi}{\Phi_Q}\theta\right), \end{aligned} \tag{9.16}$$

which is oscillatory.

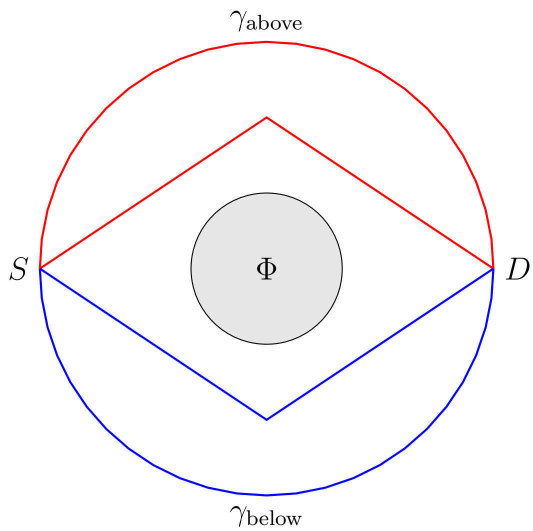

Figure 5: Aharonov Bohm effect

10 Monopoles

We usually say that $\nabla \cdot B = 0$, but if there was a magnetic monopole then

$$\nabla \cdot B = \rho m, \tag{10.1}$$

since there now a magnetic divergence. Dirac's arguments says there must be one magnetic monopole in the universe which would explain charge quantization. So if there was one magnetic monopole with strength e_m, then we would have by Gauss's law

$$\vec{B} = \frac{e_m}{r}\hat{r}, \tag{10.2}$$

and for $\vec{r} \neq 0$, we can use Stokes theorem to get

$$\vec{B} = \vec{\nabla} \times \vec{A} \implies \oint d\vec{r} \cdot \vec{A} = \int da \cdot \vec{B}. \tag{10.3}$$

So if we think of an orbit around this particle then we have that

$$E_n = \frac{\hbar^2}{2mR^2}\left(n - 2\pi\frac{\tilde{\Phi}}{\Phi_Q}\right)^2, \tag{10.4}$$

and we can calculate the flux from above and below. So we have that

$$\tilde{\Phi}_{\text{above}} - \tilde{\Phi}_{\text{below}} = 4\pi e_M = p\Phi_Q, \tag{10.5}$$

by Gauss' law. We have used the fact that the spectrum E_n must be the same above and below the monopole, in other words

$$E(\tilde{\Phi}_{\text{above}}) = E(\tilde{\Phi}_{\text{below}}), \tag{10.6}$$

and so they must differ only by the periodicity. So we know that

$$p \cdot \frac{hc}{e} = 4\pi e_m, \tag{10.7}$$

which implies the that the electron and the proton must have the same charge up to a a multiple. The charges are known to be equal to one part in 10^{19}.

11 Angular Momentum

The main point besides just understanding angular momentum is a detailed studied of symmetries. We have dealt with translational symmetry, now we will deal with rotational symmetry which is different because it is non-Abelian. This means that the

$$R_z(30) + R_z(60) = R_z(90), \tag{11.1}$$

where R_z is an abstract rotation about the z axis. On the other hand if I rotate around different axis, this is not quite true. This is important because it says that rotation cannot be written as a simple exponential as compared to momentum. So if we contrast the translation operator

$$T_x = e^{ip_x r_x/\hbar}\,;\; T_y = e^{ip_y r_y/\hbar} \tag{11.2}$$

then

$$[T_x, T_y] = 0, \tag{11.3}$$

since p_x, p_y commute. This will not be true for rotation because angular momentum is different than momentum. However, we can stil talk about generators.

11.1 Generator of Angular Momentum

11.1.1 Infinitesimal Rotations

So we will define rotation as

$$R : (V_x, V_y, V_z) \to (V'_x, V'_y, V'_z), \tag{11.4}$$

something that takes a vector to a vector with the property that R is linear and can therefore be thought of as a matrix.

$$\begin{pmatrix} V'_x \\ V'_y \\ V'_z \end{pmatrix} = R \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}, \tag{11.5}$$

with the restriction that

$$V'^2_x + V'^2_y + V'^2_z = V^2_x + V^2_y + V^2_z, \tag{11.6}$$

which implies that $RR^T = 1$, so orthogonal. So consider the rotation matrix

$$R_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{11.7}$$

, which implies that as $\phi to 0$, we have

$$\lim_{\phi\to 0} R_z(\phi) = \begin{pmatrix} 1-\phi^2/2 & -\phi & 0 \\ \phi & 1-\phi^2/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{11.8}$$

and we can calculate the rest of the infinitesimal matrices by cyclic permutation or directly. We can find that the degree away from the being commutable is

$$R_x(\phi)R_y(\phi) - R_y(\phi)R_x(\phi) = R_z(\phi^2) - I. \tag{11.9}$$

It is important to note that the order of ϕ is 2. Now we go to quantum mechanics and try to quantize this rotation operator.

11.1.2 Quantum Rotations

We know that

$$|\alpha\rangle \xrightarrow{R} D(R)\,|\alpha\rangle\,, \tag{11.10}$$

and since

$$|\beta\rangle \xrightarrow{R} D(R)\,|\beta\rangle\,, \tag{11.11}$$

we know that

$$\langle\alpha|\beta\rangle \to \langle\beta|\alpha\rangle\,, \tag{11.12}$$

which implies that $D(R)$ is unitary. So we can define a generator of rotation as

$$D(R_z(\phi)) = \exp\left(\frac{iJ_z}{\hbar}\phi\right), \tag{11.13}$$

where J_z is the angular momentum operator, which was derived analogously to the momentum translational case. By looking at rotation of vectors we realize that

$$R_x(\phi)R_y(\phi) - R_y(\phi)R_x(\phi) = R_z(\phi^2) - I, \tag{11.14}$$

which will mirror to states. So this will tell us that

$$e^{iJ_x\phi/\hbar}e^{iJ_y\phi/\hbar} - e^{iJ_y\phi/\hbar}e^{iJ_x\phi/\hbar} = e^{iJ_z\phi/\hbar} - 1, \tag{11.15}$$

which is valied for ϕ small. So if I expand both sides to order ϕ^2, I will get

$$-(J_xJ_y - J_yJ_x)\frac{\phi^2}{\hbar^2} = J_z\frac{\phi^2}{\hbar}, \tag{11.16}$$

which implies that

$$[J_x, J_y] = i\hbar J_z. \tag{11.17}$$

So the non-abelian nature of the rotation group means that there is a non-trivial commutation relation between J_i. If we add cyclic permutations, get angular momentum algebra.

11.2 Spin-1/2 as Angular Momentum

We have already seen

$$S_\alpha = \frac{\hbar}{2}\sigma_\alpha, \tag{11.18}$$

where $\alpha = x, y, z$ and σ_α are the puali matrices in the z basis. These obey the commutation relations

$$[J_x, J_y] = i\hbar J_z, \tag{11.19}$$

For example, we can put an electron,proton or neutron under a magnetic field and check that they have two energy states which are well described by rotation. So if we write a Hamiltonian as

$$H = -\gamma\vec{B}\cdot\vec{S}, \tag{11.20}$$

we know that

$$\langle H\rangle = -\gamma\vec{B}\cdot\left\langle\vec{S}\right\rangle, \tag{11.21}$$

where $\left\langle \vec{S} \right\rangle$. This thing we are measuring must be postulated to be the angular momentum. In other words, we postulate

$$D(R_z(\phi)) = \exp\left(i\frac{S_z\phi}{\hbar}\right). \tag{11.22}$$

We can check this by applying it to a state

$$D(R_z(\phi))\,|\alpha\rangle = |\alpha\rangle_R\,, \tag{11.23}$$

and look at

$$\left\langle \alpha|\vec{S}|\alpha \right\rangle_R, \tag{11.24}$$

and check that it behaves like a vector. So we must compute this expectation value which we can write as

$$\left\langle \alpha|e^{iS_z(\phi)/\hbar}S_x e^{iS_z(\phi)/\hbar}|\alpha\right\rangle. \tag{11.25}$$

We will compute this in brute force. So we have

$$\begin{aligned}\frac{\hbar}{2}e^{-iS_z\phi/\hbar}(|+\rangle\langle-| + |-\rangle\langle+|)e^{iS_z\phi/\hbar} &= \frac{\hbar}{2}\left[e^{i\phi}\,|+\rangle\langle-| + e^{-i\phi}\,|-\rangle\langle+|\right] \\ &= \cos\phi S_x - \sin\phi S_y.\end{aligned} \tag{11.26}$$

This method is simple, but only works in S_z basis with nice operators. The other way is to use Campbell-Baker-Hausdorf. Which says that

$$\begin{aligned}e^{iS_z(\phi)/\hbar}S_x e^{iS_z(\phi)/\hbar} &= S_x + \left(i\frac{\phi}{\hbar}\right)\underbrace{[S_z, S_x]}_{i\hbar S_y} + \frac{1}{2i}\left(\frac{i\phi}{\hbar}\right)^2[S_z\,\underbrace{[S_z, S_x]}_{i\hbar S_y}] + \ldots, \\ &= \cos\phi S_x - \sin\phi S_y.\end{aligned} \tag{11.27}$$

This says that our assumptions are consistent with everything else we know. In general J_α is a vector. However, when we rotate by 2π,

$$\begin{aligned}D(R_z(\phi))\,|+x\rangle &= e^{iS_z\phi/\hbar}(|+\rangle_z + |-\rangle)\frac{1}{\sqrt{2}} \\ &= \frac{e^{i\phi/2}\,|+\rangle + e^{-i\phi/2}\,|-\rangle}{\sqrt{2}} \\ &= -\,|+\rangle\,,\end{aligned} \tag{11.28}$$

when $\phi = 2\pi$. This can be observed experimentally.

11.2.1 Spin 1/2 in $\vec{B}$

In a magnetic field, the Hamiltonian becomes

$$H = -\gamma B_z S_z, \tag{11.29}$$

and we know that

$$\begin{aligned}U(t) = \exp\left(-\frac{iHt}{\hbar}\right) &= \exp\left(\frac{iS_z}{\hbar}(\gamma B_z t)\right) \\ &= D(R_z(\gamma B_z t)).\end{aligned} \tag{11.30}$$

11.2.2 Neutrons and Angular Momentum

If we make a sort of neturon interferometry experiment where there are two slits a source and a detector, we can send in spin polarized states such that all of the Neutrons start in the $|+\rangle_z$ state. On one side of one of the legs, the neutron sees a B_z field. So we are effectively performing a rotation of

$$D(R_z(\gamma B_z t)), \tag{11.31}$$

where t is the time spend in the magnetic field. So the probability of the detection is going to get

$$\begin{aligned} P &= |\langle D|S\rangle|^2 \\ &= |\langle D|S|\rangle_1 + \langle D|S\rangle_2|^2 \\ &= |\langle D|S\rangle_1 + e^{i\gamma B_z t/2}\langle D|S\rangle_2|^2 \\ &= |\langle D|S\rangle|^2 \cos^2\left(\frac{\gamma B_z t}{4}\right) \\ &= |\langle D|S\rangle|^2 \cdot \frac{1}{2}\left[1+\cos\left(\frac{\gamma B_z t}{2}\right)\right] \end{aligned} \tag{11.32}$$

where D is detector and S is the source. Notice that this is 4π periodic in $\phi = \gamma B_z t$.

11.2.3 General Rotations for Spin 1/2

Pauli matrices are 2×2 matrices with the following properties

1. $\sigma_i^2 = 1$
2. $\sigma_i\sigma_j = \sum_k i\epsilon_{ijk}\sigma_k$ for $i \neq j$.
3. $\sigma_i\sigma_j = -\sigma_j\sigma_i$ for $i \neq j$.
4. $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$.

So in the general rotation case, we have that

$$\begin{aligned} D(R_{\hat{n}}(\phi)) &= \exp\left(i\frac{\vec{S}\cdot\hat{n}}{\hbar}\phi\right) \\ &= \exp\left(i(\vec{\sigma}\dot{\vec{n}})\frac{\phi}{2}\right) \\ &= \sum_p \frac{1}{p!}\left(\frac{i\phi}{2}\right)^p (\vec{\sigma}\cdot\hat{n})^p, \end{aligned} \tag{11.33}$$

where we are working in the σ_z eigenbasis. Lets see how this works for $p = 2$,

$$\begin{aligned} (\vec{\sigma}\cdot\hat{n})^2 &= \sum_{i,j} n_i n_j \sigma_i\sigma_j \\ &= \sum_{i,j,k} n_i n_j (i\epsilon_{i,j,k}\sigma_k + \delta_{i,j} \\ &= \hat{n}\cdot\hat{n} \\ &= 1. \end{aligned} \tag{11.34}$$

So in general

$$(\vec{\sigma} \cdot \hat{n})^{\text{even}} = 1 \tag{11.35}$$

$$(\vec{\sigma} \cdot \hat{n})^{\text{odd}} = (\vec{\sigma} \cdot \hat{n}) \tag{11.36}$$

12 Orbital Angular Momentum

We know that orbital angular momentum satisfies the same algebra as angular momentum. So we know that

$$\vec{L} = \vec{x} \times \vec{p};\ [L; K_j] = i\hbar L_k \epsilon_{ijk}, \tag{12.1}$$

and we have checked that

$$L_z(z'y', z') = L_z \psi_\alpha(r, \theta, \phi) = -i\hbar \partial_\phi(r, \theta, \phi), \tag{12.2}$$

which is the generator of rotations about z. If we look at L_x, then we see that L_x generates a rotation about x and

$$L_x \psi_\alpha(x', y', z') = -i\hbar(-\sin\phi \partial_\theta - \cot\theta \cos\phi \partial\phi)\psi_\alpha(r, \theta, \phi). \tag{12.3}$$

The raising and lowering operators for orbital angular momentum are given as

$$L_\pm = -i\hbar e^{\pm i\phi} \left(\pm i\partial_\theta - \cot\theta \partial_\phi\right). \tag{12.4}$$

The other important operator is L^2. We know that $L_z = -i\hbar\partial_\phi$ so we can get that

$$L^2 = L_z^2 + \frac{1}{2}(L_+L_- + L_-L_+), \tag{12.5}$$

where the second term comes from the commutator. We can solve this as

$$L^2 = -\hbar^2 \left[\frac{1}{\sin^2\theta}\partial_\phi^2 + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta \partial_\theta\right)\right]. \tag{12.6}$$

Another way we can get at this is to notice the similarity between the Laplacian operator and go from there. This is because $p^2 = -\hbar^2\nabla^2$.

13 Spherical Harmonics

13.1 Particle in Spherical Potential

The problem is to solve for the eigenvalues of the hamiltonian which is given as

$$H = \frac{p^2}{2m} + V(|\vec{r}|). \tag{13.1}$$

where V depends only on the magnitude of r. We know the Hamiltonian is spherically symmetric which implies that

$$[L_i, H] = 0\,;\ [L^2, H] = 0\,;\ [L^2, L_z] = 0, \tag{13.2}$$

thus the eigenstates are simultaneous eigenstates of L^2 and L_z. Spherical harmonics are given as

$$Y_{lm}(\theta, \phi) = \langle \theta, \phi | l, m \rangle \,, \tag{13.3}$$

which gives that

$$L^2 Y_{lm}(\theta, \phi) = l(l+1)\hbar^2 Y_{lm}(\theta, \phi), \tag{13.4}$$

and that

$$L_z Y_{lm}(\theta, \phi) = m\hbar Y_{lm}(\theta, \phi). \tag{13.5}$$

We know that

$$\psi(r, \theta, \phi) \propto Y_{lm}(\theta\phi) = R(r) Y_{lm}(\phi, \theta), \tag{13.6}$$

since there is uniqueness of simultaneous eigenstates. So the solution must be proportional to the spherical harmonics up to a function depending only on r. Finding the form of these spherical harmonics is simular to the angular momentum case.

13.2 Properties of Y_{lm}

We know that

$$\begin{aligned}
\langle l'm' | lm \rangle &= \delta_{ll'}\delta_{mm'} \\
&= \int r^2 dr \, \sin\theta d\theta d\phi \psi^*_{l'm'}(r, \theta, \phi)\psi_{lm}(r, \theta, \phi) \\
&= r^2 dr \, R_\alpha(\vec{r}) R_\beta(\vec{r}) \int \sin\theta \, d\theta d\phi Y^*_{lm}(\theta, \phi) Y_{lm}(\theta, \phi) \\
&= \int_0^\pi \sin\theta \, d\theta \int_{-\pi}^{\pi} d\phi Y^*_{lm}(\theta, \phi) Y_{lm}(\theta, \phi) \\
&= \delta_{ll'}\delta_{mm'},
\end{aligned} \tag{13.7}$$

and we can act with L_z to get that

$$-i\hbar\partial_\phi Y_{lm}(\theta, \phi) = m\hbar Y_{lm}(\theta, \phi), \tag{13.8}$$

which implies that

$$Y_{lm}(\theta, \phi) = e^{im\theta} Y_{lm}(\theta, \phi). \tag{13.9}$$

So we can use the raising operator to get that

$$\begin{aligned}
L_+ Y_{lm}(\theta, \phi) &= 0 \\
\implies -i\hbar e^{i\theta} \left(i\partial_\theta - \cot\theta \partial_\phi \right) Y_{ll}(\theta, \phi) &= 0 \\
\implies \left(i\partial_\theta - il\cot\theta \right) Y_{ll}(\theta, \phi) &= 0 \\
\implies \left(\partial_\theta - \frac{l\cos\theta}{\sin\theta} \right) Y_{ll}(\theta, \phi) &= 0
\end{aligned} \tag{13.10}$$

which implies that

$$Y_{ll}(\theta, \phi) \propto \sin^l\theta. \tag{13.11}$$

So in general, we have that

$$Y_l^m(\theta, \phi) = C(-1)^l e^{im\phi} \frac{1}{\sin^m\theta} \frac{d^{l-m}}{d(\cos\theta)^{l-m}} \sin^{2l}\theta, \tag{13.12}$$

where C is a constant.

All this is technically only true for $m \geq 0$, and so if we do not have this condition, for $m \leq 0$, we can define

$$y_l^m(\theta, \phi) \rightarrow y_l^{-m^*}(\theta, \phi), \tag{13.13}$$

which is still a valid solution.

There are two special cases that are interesting. The spherical harmonics for $m = 0$ are the Legendre Polynomials and also that for $m > 0$,

$$Y_l^m(\theta = 0, \phi) = 0, \tag{13.14}$$

since there cannot be a ϕ dependence for something on the z axis.

13.3 Quantization

We can find quantization conditions on m, l. We know that the wave function is periodic

$$Y_l^m(\theta, \phi + 2\pi) = Y_l^m(\theta, \phi), \tag{13.15}$$

which implies

$$e^{2\pi i m} = 1, \tag{13.16}$$

so m is an integer. in fact $m = l, l-1, \ldots, -l$, which is also an integer. This integer quantization is true for orbital angular momentum since it generates rotations for coordinates. This same quantiziation is not true for regular angular momentum. In general it is either integer or half integer. Usually if there is a coordinate degree of freedom, it is integer.

13.4 Connection to Wigner D Matrices

We can write the spherical harmonics as

$$Y_{lm}(\theta, \phi) = \langle \theta, \phi | l, m \rangle = \langle \hat{n} | l, m \rangle . \tag{13.17}$$

We can write $|\hat{n}\rangle$ as

$$|\hat{n}\rangle = D(R) |\hat{z}\rangle , \tag{13.18}$$

a rotation about the z axis. So we can also see that by indtroducing a complete set of states

$$\begin{aligned} Y_{lm}^*(\theta, \phi) = \langle lm | \hat{n} \rangle &= \langle lm | D(R(\theta, \phi, 0)) | \hat{z} \rangle \\ &= \sum_{m'} \underbrace{\langle lm | D(R) | lm' \rangle}_{D^{(l)}_{mm'}(R)} \underbrace{\langle lm' | \hat{z} \rangle}_{\delta_{m',0} Y_{l0}(\theta=0)} \\ &= D^{(l)}_{m0}(R(\theta, \phi, 0)) Y_{l0}(\theta = 0). \end{aligned} \tag{13.19}$$

So noting that

$$Y_{l0}(\theta = 0) = \sqrt{\frac{2l+1}{4\pi}} \tag{13.20}$$

we can see that

$$D^{(l)}_{m0}(R(\theta, \phi, 0)) = \sqrt{\frac{4\pi}{2l+1}} Y_{lm}^*(\theta, \phi). \tag{13.21}$$

14 Radial Equation

We are interesting in solving problems with Hamiltonians of the form

$$H = \frac{p^2}{2m} + V(|\hat{r}|), \tag{14.1}$$

and we will use L_z, L^2 to note that we can write the equation as

$$R_{nlm}(r)Y_{lm}(\theta, \phi), \tag{14.2}$$

a separation of variables. We have already looked at the spherical harmonics, so now we look at the radial part. So we want to solve the Shrodinger equation

$$H\psi_{nlm}(r, \theta, \phi) = E\psi_{nlm}(r, \theta, \phi). \tag{14.3}$$

Which we can rewrite in this case as

$$\frac{1}{2m}p^2\psi_{nlm} + V(|r|)\psi_{nlm} = E\psi_{nlm}. \tag{14.4}$$

Breaking this up into parts, we note that

$$p^2\psi(r, \theta, \phi) = \frac{1}{2mr^2}L^2\psi(r, \theta, \phi) - \frac{\hbar^2}{2mr^2}\partial_r(r^2\partial_r)\psi(r, \theta, \phi), \tag{14.5}$$

which we found by looking at $L = \hat{x} \times \hat{p}$ and L^2. So we can substitute this and use the fact that

$$L^2 Y_{lm}(\theta, \phi) = l(l+1)\hbar^2 Y_{lm}(\theta, \phi), \tag{14.6}$$

we get that

$$-\frac{\hbar^2}{2mr^2}\left[\partial_r(r^2\partial_r R(r))\right] Y_{lm}(\theta, \phi) + \frac{1}{2mr^2}R(r)l(l+1)\hbar^2 Y_{lm}(\theta, \phi) + (V(r) - E)R(r)Y_{lm}(\theta, \phi), \tag{14.7}$$

but we can cancel out the shperical harmonics to get that

$$-\frac{\hbar^2}{2mr^2}\left[\partial_r(r^2\partial_r R(r))\right] + \left(\frac{1}{2mr^2}l(l+1)\hbar^2 + V(r) - E\right) R(r). \tag{14.8}$$

We want to transform this into the 1D shrodinger equation, which we know how to solve. So we can write make a substitution of variables

$$R(r) = \frac{u(r)}{r}, \tag{14.9}$$

which transforms the equation into

$$-\frac{\hbar^2}{2m}\partial_r^2 u + V_{eff}(r)u = Eu, \tag{14.10}$$

where

$$V_{eff} = V(r) = \frac{l(l+1)\hbar^2}{2mr^2}, \tag{14.11}$$

which is a 1D Schrodinger equation except that there is a term dependant on l which takes into account the angular momentum part of the problem. It is like a central barrier.

14.1 Normalization

We know that

$$\int r^2 \sin\theta |\psi(r,\theta,\phi)|^2 \, dr d\theta d\phi = 1, \tag{14.12}$$

which only becomes a normalization conditions if $R(r) = u(r)/r$. This is a good way to remember the form.

14.2 Solutions

If we attempt to solve the equation

$$\partial_l^2 y = \frac{-l(l+1)}{2mr^2} u, \tag{14.13}$$

we can find the solution as

$$u(r) = Ar^{l+1} + Br^{-l}. \tag{14.14}$$

B must be zero or we cannot normalize the wave function since

$$\int_0^\infty dr u(r)^2 \sim B^2 \int_0^\infty dr \, r^{-2l} \tag{14.15}$$

and therefore it is not part of the Hilbert space. So this means that $B = 0$. As $r \to \infty$, then if $V(r)$ also goes to zero, we get the free particle Hamiltonian which we know how to solve. If we are solving for a bound state, then

$$E = -\frac{\hbar^2}{2m}\kappa^2 < 0, \tag{14.16}$$

which implies that $u \propto e^{-\kappa r}$. So we have the two limits. Sometimes it is convenient to take out these two singularities (long and short distance) and we want define

$$u = r^{l+1} e^{-\kappa r} w(r), \tag{14.17}$$

where $w(r)$ is well behaved. This can be convenient in some situations.

14.2.1 Some Notes

- l is the eigenvalue of the L^2 operator and m of the L_z operator.
- We make the substitution to u and can solve the problems.

14.3 Spherical Well

So we now define

$$V_{eff}(r) = V(r) + l(l+1)\frac{\hbar^2}{2mr}, \tag{14.18}$$

as before and for the spherical well we define

$$V(r) = \begin{cases} 0 & r < a \\ \infty & r \geq a. \end{cases} \tag{14.19}$$

So we need to solve for $r < a$ and set $u(r = a)$ to be zero. So the Shrodinger equation becomes

$$-\frac{\hbar^2}{2m}u'' + \frac{l(l+1)}{2mr^2}u = Eu, \tag{14.20}$$

which is not easy to solve for general l. However, for $l = 0$, we can solve it relatively easy. The equation then becomes

$$-\frac{\hbar^2}{2m}u'' = \frac{\hbar^2 k^2}{2m}u, \tag{14.21}$$

where $E = \hbar^2 k^2/2m$. So this means that

$$u(r) = A\sin(kr) + B\cos(kr). \tag{14.22}$$

Since $U(r) \propto r$ at small r, we can set B to zero. So now we note that at

$$u(a) = \sin(ka) = 0, \tag{14.23}$$

which quantizes k as $k = n\pi/a$, so our bound states are

$$u_n(r) = \sin\left(\frac{n\pi}{a}r\right). \tag{14.24}$$

and

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \tag{14.25}$$

For $l \neq 0$, we can write our equation in terms of r and get

$$-\frac{\hbar^2}{2m}\partial_r(rR) + l(l+1)\frac{\hbar^2}{2mr^2}rR = \frac{\hbar^2 k^2}{2m}rR \tag{14.26}$$

and after canceling and setting $kr = x$, we get

$$-\frac{1}{x}\partial_x^2(xR) + \frac{l(l+1)}{x^2}R = R, \tag{14.27}$$

which is the spherical Bessel equation. So $R(x)$ has solution

$$R(x) = AJ_l(x) + BN_l(x), \tag{14.28}$$

which means we get that

$$R(r) = AJ_l(kr) + BN_l(kr), \tag{14.29}$$

by using our substitution for x. As $r \to 0$, we need the functions need to go to r^l. Since $N_l(x)$ asymptotes to an incorrect value $B = 0$. So up to a constant

$$R(r) = J_l(kr), \tag{14.30}$$

and we can solve using the boundary condition at a. We can find quantization conditions by looking at the zeros of the Bessel functions which are known.

14.4 Harmonic Potential

In this case, the potnential is given as

$$V(r) = \frac{1}{2}m\omega^2 r^2, \tag{14.31}$$

and so

$$V_{eff} = \frac{1}{2}m\omega^2 r^2 + \frac{l(l+1)\hbar^2}{2mr^2}. \tag{14.32}$$

For $l = 0$ this is the simple harmonic oscillator with only a slight difference. We need to satisfy the boundary condition at the origin, which means that $u(r \to 0) \propto r^{l+1} = r$ for the case of $l = 0$. The result is that only odd n are allowed for $l = 0$. So

$$u_n(r) = \phi_{1D,2n+1}(r), \tag{14.33}$$

since we must have nodes at 0. So now we have all the eigenstates and eigenvalues for $l = 0$.

As $r \to \infty$, for any l, we can approximate $V_{eff}(r)$ will be dominated by $\frac{1}{2}m\omega^2 r^2$ and so our approximated Shrodinger equation becomes

$$-\frac{\hbar^2}{2m}u'' \approx -\frac{1}{2}m\omega^2 r^2 u, \tag{14.34}$$

which we can solve as

$$u(r) \propto \exp\left[-\frac{1}{2}\left(\frac{m\omega}{\hbar}\right)r^2\right]. \tag{14.35}$$

We can also solve the equation at finite l and this is shown in Sakurai. But we are going to do it slightly different. One interesting fact is that the radial equation eigenvalues are independent of m due to rotational symmetry. So

$$E_{nlm} = E_{nl}. \tag{14.36}$$

We will take an operator approach. We can write the 3D harmonic oscillator as

$$H = \sum_j \left(\frac{p_j^2}{2m} + \frac{1}{2}m\omega^2 x_j^2\right), \tag{14.37}$$

where $j = 1, 2, 3$, $r^2 = x_1^2 + x_2^2 + x_3^2$. So $x, y, z = x_1, x_2, x_3$. Since we also know that

$$[x_j, P_k] = i\hbar\delta_{jk}, \tag{14.38}$$

so we can write

$$H = H_1 + H_2 + H_3, \tag{14.39}$$

where

$$H_j = \frac{p_j^2}{2m} + \frac{1}{2}\omega^2 x_j^2, \tag{14.40}$$

and so we can solve by definiting a bunch of creation operators and annhiliation operators as

$$a_j^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x_j - \frac{ip_j}{m\omega}\right) \tag{14.41}$$

and we could define

$$\hat{n} = a_j^\dagger a_j, \tag{14.42}$$

and then we could solve for the energy as

$$E(n_1, n_2, n_3) = \hbar\omega \left(n_1 + n_2 + n_3 + \frac{3}{2} \right). \tag{14.43}$$

However although we have symmetry and

$$[H, L^2] = [H, L_z] = 0, \tag{14.44}$$

our eigenfunctions

$$|n_1, n_2, n_3\rangle \propto a_1^{\dagger n_1} a_2^{\dagger n_2} a_3^{\dagger n_3} |0\rangle, \tag{14.45}$$

are not eigenstates of L^2 and L_z and so they change under rotation. So we cannot say anything about what happens if you rotate this states. This could be necessary if you needed to do perturbation theory. So we want to know the value of

$$\langle Q, lm | n_1, n_2, n_3 \rangle. \tag{14.46}$$

So we will need to go into this other basis So we need to diagonalize in the l, m basis. Since the radial approach is not easy, we will use this other way. The answer is buried in the observation that there is a $U(3)$ symmetry "hidden" in the 3D harmonic oscillator. In the "Cartesian" basis there was a symmetric form the the Hamiltonian as

$$H = \hbar\omega \left(\sum_j a_j^\dagger a_j + \frac{3}{2} \right) \tag{14.47}$$

So we can transform

$$a_j \mapsto \sum_k U_{jk} a_k = a_j. \tag{14.48}$$

So we can write

$$A = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \tag{14.49}$$

and then

$$A' = \begin{pmatrix} a_1' \\ a_2' \\ a_3'' \end{pmatrix} = UA, \tag{14.50}$$

which gives rise to our Hamiltonian as

$$H = \hbar\omega \left(A^\dagger A + \frac{3}{2} \right) = \hbar\omega \left(A'^\dagger U U^\dagger A' + \frac{3}{2} \right) = \hbar\omega \left(A'^\dagger A' + \frac{3}{2} \right), \tag{14.51}$$

and so

$$[a_j, a_k^\dagger] = \delta_{jk} = [A, A^\dagger]_{jk}, \tag{14.52}$$

which we now look at the matrix elements of operatation by the unitary matrix as

$$(U^\dagger [A, A'^\dagger] U)_{jk} = \delta_{jk}, \tag{14.53}$$

which implies that

$$[a'_j, a'^{\dagger}_k] = \delta_{jk}, \tag{14.54}$$

so this is a canonical transformation. Since U is a three by three unitary matrix, this is a $U(3)$ symmetry of the harmonic oscillator. This is not necessarily obvious, but it will be useful in solving the equation. So we can write

$$U = e^{i\phi}\tilde{U}, \tag{14.55}$$

and construct generalized angular momentum for any U. However, we will choose a U that we "like" in the sense that it will be easy to solve. So we choose U as

$$\begin{pmatrix} a'_1 \\ a'_2 \\ a'_3 \end{pmatrix} = U \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} (a_1 + ia_2)/\sqrt{2} \\ (a_1 - ia_2)/\sqrt{2} \\ a_3 \end{pmatrix} \tag{14.56}$$

so we have the operators

$$a_{\pm} = \frac{a_1 \mp ia_2}{\sqrt{2}} \tag{14.57}$$

$$a_0 = a_3, \tag{14.58}$$

Now we will switch backto x, y, z notation as and so we have that

$$a^{\dagger}_{\pm} = \frac{a^{\dagger}_x \pm ia^{\dagger}_y}{\sqrt{2}} \tag{14.59}$$

$$a^{\dagger}_0 = a^{\dagger}_z, \tag{14.60}$$

$$e^{iL_z\phi}a^{\dagger}_1 e^{-iL_z\phi} = \cos\phi a^{\dagger}_1 + \sin\phi a^{\dagger}_2, \tag{14.61}$$

which is a special case of Tensor operators. The nice thing about the operators we have defined is that we can after some algebra get that

$$e^{iL_z\phi}a^{\dagger}_{\pm}e^{-iL_z\phi} = e^{i\phi}a^{\dagger}_{\pm}, \tag{14.62}$$

and a_0 will be invariant since the z direction will not be transformed by a rotation about the z axis. So now that we have defined these useful operators, we will write our hamiltonian as

$$H = \hbar\omega\left(a^{\dagger}_0 a_0 + a^{\dagger}_+ a_+ + a^{\dagger}_- a_- + \frac{3}{2}\right), \tag{14.63}$$

and by solving this basis, we also have that

$$H\left|n_+, n_-, n_0\right\rangle = \hbar\omega\left(n_+, n_- + n_0 + \frac{3}{2}\right), \tag{14.64}$$

but this is an eigenstate of L_z which we can see by applying rotation operators to this state since

$$\left|n_+, n_-, n_0\right\rangle \propto a^{\dagger n_+}_+ a^{\dagger n_-}_- a^{\dagger n_0}_0 \left|0\right\rangle \tag{14.65}$$

and so when we apply the rotation operators we get that

$$e^{iL_z\phi}\left|n_+, n_-, n_0\right\rangle \propto e^{iL_z\phi}a^{\dagger n_+}_+ a^{\dagger n_-}_- a^{\dagger n_0}_0 e^{-iL_z\phi}\left|0\right\rangle \tag{14.66}$$

and to avoid degeneracy (the lowest state is $n_i = 0$. So we know for $|0\rangle$, $L^2 = L_z = 0$. This gives rise to

$$e^{i(n_+ - n_-)\phi} |n_+, n_-, n_0\rangle \tag{14.67}$$

So we can compare and get

$$L_z = M\hbar = (n_+ - n_-)\hbar, \tag{14.68}$$

which will allow us to take our previous result that

$$E = \hbar\omega \left(N + \frac{3}{2} \right), \tag{14.69}$$

where $N = n_0 + n_+ + n_-$ and $n \in \mathbb{Z}_+$. So know that since the M are also integer, we can combine equations and get that

$$n_+ = \frac{N - n_0 + M}{2} \leq N \tag{14.70}$$

$$n_- = \frac{N - n_0 - M}{2} \geq 0, \tag{14.71}$$

which implies that n_0 has the same parity as $N \pm M$, which means that

$$(-1)^{n_0} = (-1)^N (-1)^M \tag{14.72}$$

So $n_0 \leq N - M$ and $n_0 \geq M$. What this says is that there are $N/2 - M$ states. So if N and M are even,

$$n_0 = M, M+2, \ldots, N - M \tag{14.73}$$

We can think about this as a table with n_+ on one axis and n_- on the other axis with n_+ running from $0 \to N$ upwards on the y axis and n_- running from $0 \to N$ right on the x axis meeting at the top left. We can then find the allowed states and the not allowed states. We can immediatly see that $L \leq N$. So the main result is that the allowed L are

$$L = N, N-2, N-3, \ldots 0 \tag{14.74}$$

and

$$M = -L, \ldots, L, \tag{14.75}$$

for each N.

14.4.1 Harmonic Oscillator Summary

The takeaway from the last time as that we can write the energy as

$$E(n_x, n_y, n_z) = \hbar\omega \left(\underbrace{n_x + n_y + n_z}_{N} + \frac{3}{2} \right), \tag{14.76}$$

but we can use a different basis $|l, m, q\rangle$ and we still have the same energy, but the allowed angular momenta

$$l = N, N-2, \cdots \geq 0. \tag{14.77}$$

So we notice that l, N have the same parity and we will explain this later. It has to do with reflection symmetry. One check that we can do to remember this (it has been expected on a qualifier problem before) would be to count dimension. So for $N = 3$, we will count in two basis. In the Cartesian basis, it is the combination of n_i such that $N = 3$. And in terms of l, we can have $l = 3$ corresponding to $2l + 1$ or 7 states and $l = 1$ which corresponds to 3 states. So there are ten states allowed.

14.5 Review of $r \to 0$ Boundary Condition

For $l > 0$ as $r \to 0$ if we look at the solution

$$u = Ar^{l+1} + Br^{-l}, \tag{14.78}$$

we must have that $B = 0$ for normalizability reasons. At $l = 0$, B still must go to 0, however, it is for a different reason and Sakurai's argument is not really good. So if we look at

$$\psi(r) = \frac{u}{r} = A = \frac{B}{r}, \tag{14.79}$$

but we know that ψ is a solution of the Schrodinger equation. So if we plug in, then A contributes zero and B contributes a δ function by analogy to a potential of an electrostatic potential. So we get the equation

$$-B\delta^3(r) + V\psi = E, \tag{14.80}$$

which is a contradiction since a delta function is singular in a way that V, E are not. So therefore, B must be zero.

14.6 Hydrogen Atom

We are going to do the SO(4) solution. So we have that the Hamiltonian is given as

$$H = \frac{p^2}{2m} - \frac{Ze^2}{|\vec{r}|}, \tag{14.81}$$

and we know that L^2 and L_z commute with the Hamiltonian as in any central force problem, as is the Lenz vector which is defined as

$$\vec{M} = \frac{\vec{p} \times \vec{L}}{m} - \frac{Ze^2}{r}\vec{r}. \tag{14.82}$$

This is the classical form and to make it quantum, we need to symmetrize it as

$$\vec{M} = \frac{1}{2m}\left(\vec{p} \times \vec{L} - \vec{L} \times \vec{p}\right) - \frac{Ze^2}{r}\vec{r}. \tag{14.83}$$

Now we can see that

$$\vec{L} \cdot \vec{M} = 0, \tag{14.84}$$

and also that

$$M^2 = \frac{2}{m}H(L^2 + \hbar^2) + Z^2e^4. \tag{14.85}$$

So now we need to figure out the algebra between L and M. The algebra comes from Wigner-Echart and has the algebra

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{14.86}$$

$$[M_i, L_j] = i\hbar\epsilon_{ijk}M_k \tag{14.87}$$

$$[M_i, M_j] = -i\hbar\epsilon_{ijk}\frac{2H}{m}L_k. \tag{14.88}$$

These all turn out to be special cases of poisson brackets and the general formulation of making a classical operator quantum. We can see the third relation is different than the other two. So we can focus on the energy eigenspace of bound states $E < 0$, and so we can define

$$N_i = M_i\sqrt{\frac{-m}{2E}}, \tag{14.89}$$

which gives commutation relations as

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{14.90}$$

$$[N_i, L_j] = i\hbar\epsilon_{ijk}N_k \tag{14.91}$$

$$[N_i, N_j] = i\hbar\epsilon_{ijk}L_k, \tag{14.92}$$

which is a nicer form. Now we can see that this is SO(4), since if we look at coordinates x_j, p_j for $j = 1, 2, 3, 4$, then the natural definition is

$$\tilde{L}_{ij} = x_i p_j - x_j p_i \tag{14.93}$$

We can see that this would imply

$$\begin{aligned} \tilde{L}_{12} &= L_z \\ \tilde{L}_{23} &= L_x \\ \tilde{L}_{31} &= L_y \\ \tilde{L}_{14} &= N_x \\ \tilde{L}_{24} &= N_y \\ \tilde{L}_{34} &= N_z, \end{aligned} \tag{14.94}$$

which would generate the proper commutation relations. This says that we can map the way rotation usually looks to these specific commuations and so this is S0(4). The interesting feature is that SO(4) is not irreducible, so it can be broken up into three copies of SO(3), we can see this by defining

$$I = \frac{L+N}{2} \tag{14.95}$$

$$J = \frac{L-N}{2}, \tag{14.96}$$

then the commutation relations decouple and we left with

$$[I_i, I_j] = i\hbar\epsilon_{ijk}I_k \tag{14.97}$$

$$[K_i, K_j] = i\hbar\epsilon_{ijk}K_k \tag{14.98}$$

$$[I_i, K_j] = 0, \tag{14.99}$$

which means we can just look at simultaneous eigenstates of the normal angular momentum algebra and look at simultaneous eigenkets of I^2, I_z, K^2, K_z which satisfy the constraint

$$I^2 - K^2 = (I - K) \cdot (I + K) = 0, \tag{14.100}$$

which implies that $I^2 = K^2$. So we know that $K^2 = k(k+1)\hbar^2$ and $I^2 = i(i+1)\hbar^2$, and we know that

$$K_z, I_z = -k, \dots, k, \tag{14.101}$$

so there are $(2k+1)^2$ degenerate values. Now notice that

$$\begin{aligned} I^2 + K^2 &= \frac{L^2 + N^2}{2} \\ &= \frac{1}{2}\left(L^2 - \frac{m}{2E}M^2\right) \\ &= 2k(k+1)\hbar^2. \end{aligned} \tag{14.102}$$

We also have the other equation

$$M^2 = \frac{2E}{m}(L^2 + \hbar) + Z^2 e^4, \tag{14.103}$$

and by combining our equations, we get that

$$E_k = -\frac{mZ^2e^4}{2\hbar^2(2k+1)^2}, \tag{14.104}$$

where $k = 0, 1/2, 1, 3/2, 2, \dots$ and we can also solve the the allowed L^2 as

$$L \leq 2k + 1. \tag{14.105}$$

This also gives us the orbital degeneracies directly. For example if $k = 0$, we can only have $l = 0$, so there is only the 1s state.

15 Addition of Angular Momentum

To illustrate this, we will put a spin 1/2 particle in a spherical potential. First we want to look at the Hilbert space. We have a tensor product representation of spin and position

$$|\vec{x}\rangle \otimes |\pm\hbar/2\rangle\,, \tag{15.1}$$

and so the wavefunction for sum state α is given as

$$\langle x; \pm|\alpha\rangle\,, \tag{15.2}$$

where $m_x = \pm 1/2$ and is the eigenvalue of the spin operator S_z. In this space, the operator is really

$$\vec{S} = 1 \otimes \vec{S}, \tag{15.3}$$

as it only acts on the spin part of the Hilbert space. On the hand, we also have the orbital angular momentum operator L which is given by

$$\vec{L} = \vec{L} \otimes 1. \tag{15.4}$$

In terms of the wavefunctions, this tells us that

$$\left\langle x; m_s|\vec{L}|\alpha\right\rangle = \vec{L}\psi_{m_s}(\vec{x}), \tag{15.5}$$

and we also have that

$$\begin{aligned}\left\langle x; m_s|\vec{S}|\alpha\right\rangle &= \sum_{m_s'}\int \left\langle xm_s|\vec{S}|x'm_s'\right\rangle \langle x'm_s'|\alpha\rangle \\ &= \sum_{m_s'}\left\langle m_s|\vec{S}|m_s'\right\rangle \psi_{m_s'}(x)\end{aligned} \tag{15.6}$$

and so we can write this as a spinor wavefunction as

$$\psi(x) = \begin{pmatrix}\psi_+(\vec{x})\\ \psi_-(\vec{x})\end{pmatrix} \tag{15.7}$$

which we can use to write

$$\vec{L}\psi(x) = \begin{pmatrix}L\psi_+(x)\\ L\psi_-(x)\end{pmatrix} \;;\; \vec{S}\psi(x) = S\begin{pmatrix}\psi_+(\vec{x})\\ \psi_-(\vec{x})\end{pmatrix} \tag{15.8}$$

However, we should not be working in the position basis, instead we should expand in terms of radial eigenstates. So we have that

$$\psi_{m_s}(\vec{x}) = \sum_{n,l,m_l} R_n(r)Y_{lm_l}(\theta,\phi) = \sum_{n,l,m_l}\psi_{lm_lm_s}(r,\theta,\phi), \tag{15.9}$$

which allows us to write that

$$L_z\begin{pmatrix}\psi_{lm_l+}(\theta,\phi)\\ \psi_{lm_l-}(\theta,\phi)\end{pmatrix} = m_l\hbar\begin{pmatrix}\psi_{lm_l+}(\theta,\phi)\\ \psi_{lm_l-}(\theta,\phi)\end{pmatrix} \tag{15.10}$$

so these wavefunctions are eigenstates of L_z and there are eigenstates of L^2 given as

$$L^2\begin{pmatrix}\psi_{lm_l+}(\theta,\phi)\\ \psi_{lm_l-}(\theta,\phi)\end{pmatrix} = l(l+1)\hbar^2\begin{pmatrix}\psi_{lm_l+}(\theta,\phi)\\ \psi_{lm_l-}(\theta,\phi)\end{pmatrix} \tag{15.11}$$

For the S_z operator, we have that

$$S_z\begin{pmatrix}\psi_{lm_l+}(\theta,\phi)\\ 0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}\psi_{lm_l+}(\theta,\phi)\\ 0\end{pmatrix} \tag{15.12}$$

and also that

$$S_z\begin{pmatrix}0\\ \psi_{lm_l-}(\theta,\phi)\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}0\\ \psi_{lm_l-}(\theta,\phi)\end{pmatrix} \tag{15.13}$$

So the upshort of this is that we can write the following

$$\langle r,\theta,\phi; l, m_l, +\rangle = \begin{pmatrix}\psi_{lm_l+}(r,\theta,\phi)\\ 0\end{pmatrix} \tag{15.14}$$

and also that

$$\langle r,\theta,\phi; l, m_l, -\rangle = \begin{pmatrix}0\\ \psi_{lm_l-}(r\theta,\phi)\end{pmatrix} \tag{15.15}$$

so with this basis, we have both eigenstates of L_z and S_z, and L^2 in the following sense

$$L_z\left|lm_l\pm\right\rangle = m_l\hbar\left|lm_l\pm\right\rangle \tag{15.16}$$

$$S_z\left|lm_l\pm\right\rangle = \pm\frac{\hbar}{2}\left|lm_l\pm\right\rangle \tag{15.17}$$

$$L^2\left|lm_l\pm\right\rangle = l(l+1)\hbar^2\left|lm_l\pm\right\rangle. \tag{15.18}$$

15.1 Rotation Operators

We can define a rotation operator as

$$D(R)\left(|l, m_l\rangle \otimes |\pm\rangle\right) = \left(D^{orb}(R)\,|l, m_l\rangle\right) \otimes \left(D^{spin}(R)\,|\pm\rangle\right)$$
$$= \exp\left(-i(\vec{L}\cdot\vec{n})\frac{\phi}{\hbar}\right)\exp\left(-i(\vec{S}\cdot\vec{n})\frac{\phi}{\hbar}\right)$$
$$\exp\left(-i((\vec{L}+\vec{S})\cdot\vec{n})\frac{\phi}{\hbar}\right)$$
$$= \exp\left(-i(\vec{n}\cdot\vec{J})\frac{\phi}{\hbar}\right), \tag{15.19}$$

where

$$\vec{J} = \vec{L} + \vec{S}. \tag{15.20}$$

So the problem becomes how to relate the eigenstates of J to this new basis. So we need to get

$$|j, m\rangle \mapsto |m, m_l, m_s\rangle\,. \tag{15.21}$$

The coefficients when one expands into this basis are called the Clebsch-Gordon coefficients.

15.2 $S = 1/2$ Case

So we know that

$$J_z = L_z + S_z, \tag{15.22}$$

and assume that l is fixed since L^2 and J commute. So we ant to find

$$|j, m\rangle = \sum_{m_l, m_s} C_{m_l, m_s}\,|l, m_l, m_s\rangle\,, \tag{15.23}$$

which leads to

$$J_z\,|j, m\rangle = \sum_{m_l, m_s} C_{m_l, m_s}(L_z + S_z)\,|l, m_s, m_s\rangle = m\hbar\,|j, m\rangle\,, \tag{15.24}$$

which implies that

$$m = m_l + m_s. \tag{15.25}$$

So for spin 1/2, we have that

$$|j, m\rangle = (C_+^{(j)}\underbrace{|l, m_l = m - 1/2; 1/2\rangle}_{|A\rangle} + C_-^{(j)}\underbrace{|l, m_l = m + 1/2; -1/2\rangle}_{|B\rangle}\,. \tag{15.26}$$

Since we know that this must be an eigenstate of J^2, we must have that

$$J^2\,|j, m\rangle = \hbar^2 j(j+1)\,|j, m\rangle\,, \tag{15.27}$$

and so we can write

$$J^2 = (L+S)^2 = L^2 + S^2 + L_z S_z + \frac{1}{2}(L_+ S_- + L_- S_+). \tag{15.28}$$

we can then combine to get that

$$\begin{pmatrix} \langle A|J^2|j,m\rangle \\ \langle B|J^2|j,m\rangle \end{pmatrix} = \hbar^2 j(j+1) \begin{pmatrix} C_+^{(j)} \\ C_-^{(j)} \end{pmatrix}, \tag{15.29}$$

as well as

$$\begin{pmatrix} \langle A|J^2|j,m\rangle \\ \langle B|J^2|j,m\rangle \end{pmatrix} = \begin{pmatrix} \langle A|J^2|A\rangle & \langle A|J^2|B\rangle \\ \langle B|J^2|A\rangle & \langle B|J^2|B\rangle \end{pmatrix} \begin{pmatrix} C_+^{(j)} \\ C_-^{(j)} \end{pmatrix}, \tag{15.30}$$

which is the standard eigenvalue problem and we can get the final rule which is that

$$j = l \pm \frac{1}{2} \tag{15.31}$$

where the the equation is given as 3.8.64. We can get this by Clebsch-Gordon, but it also works this way. We give the corresponding wavefunctions as

$$j = l + \frac{1}{2} \to \begin{pmatrix} \sqrt{\frac{l-m+1/2}{2l+1}} \\ \sqrt{\frac{l+m+1/2}{2l+1}} \end{pmatrix}, \tag{15.32}$$

and

$$j = l - \frac{1}{2} \to \begin{pmatrix} \sqrt{\frac{l+m+1/2}{2l+1}} \\ -\sqrt{\frac{l-m_1/2}{2l+1}} \end{pmatrix} \tag{15.33}$$

15.2.1 Application

If the Hydrogen atom Hamiltonian was

$$H = H_0 + \gamma \vec{L} \cdot \vec{S} \tag{15.34}$$

The second term commutes with J^2 and is called spin-orbit coupling. However, $|l, m_l\rangle \otimes |m_s\rangle$ does not diagonalize the Hamiltonian, but the $|j, m\rangle$ basis does. Now we can use the fact that

$$\vec{L} \cdot \vec{S} = \frac{\vec{J}^2 - \vec{L}^2 - \vec{S}^2}{2}, \tag{15.35}$$

to calculate the eigenvalues. We finally calculate that

$$E = E_n + \hbar^2 \gamma \left[\frac{j(j+1) - l(l+1) - 3/4}{2} \right] \tag{15.36}$$

15.2.2 Pair of spin-1/2

If we instead have the Hamiltonian

$$H = \gamma \vec{S}_1 \cdot \vec{S}_2, \tag{15.37}$$

then we have the options $j = 1/2 - 1/2 = 0$ (singlets) and $j = 1/2 + 1/2 = 1$ (triplet). This is because $j = 0$ is non-degenerate, so $m = 0$, and the only state is

$$\frac{1}{\sqrt{2}} \left(\left| \frac{1}{2} \right\rangle \otimes \left| -\frac{1}{2} \right\rangle - \left| -\frac{1}{2} \right\rangle \otimes \left| \frac{1}{2} \right\rangle \right) \tag{15.38}$$

and the eigenvalue is

$$E = -\frac{3}{4}\hbar^2\gamma \tag{15.39}$$

(we have used the relation for S in terms of J^2. So for the triplet states, there are three degenerate states and the general formula is givne as

$$E = \frac{\hbar}{2}(j(j+1) - 3/4 \cdot 2)\gamma, \tag{15.40}$$

which implies in this case

$$E = \gamma\frac{\hbar^2}{4} \tag{15.41}$$

15.3 General Angular Momentum Addition

For the general case, we have

$$\underbrace{|j_1, m_1\rangle}_{J_1} \otimes \underbrace{|j_2, m_2\rangle}_{J_2}, \tag{15.42}$$

we want to look at eigenstates of the total angular momentum

$$\vec{J} = \vec{J_1} + \vec{J_2}, \tag{15.43}$$

which are $|j, m\rangle$ where $m = m_1 + m_2$. The Clebsch-Gordon coefficients are a way to go between these two basis. Usually we will use the notmation $|j_1 j_1; m_1 m_1\rangle$ for the first way and $|j_1 j_2; jm\rangle$ for the second basis. So we can insert a complete set of states as

$$|j_1 j_2; jm\rangle = \sum_{m_1 m_1} |j_1 j_2; m_1 m_2\rangle \underbrace{\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle}_{CBCoef} \tag{15.44}$$

These coefficients have the following properties

- $\langle j_1 j_1; m_1 m_2 | j_1 j_2; jm\rangle \propto \delta_{m, m_1+m_2}$
- They are only non zero if $|j_1 - j_2| \leq j \leq |j_1 + j_2|$ This is the classical triangle inequality.

We also know that

$$J_\pm |j_1 j_2; jm\rangle = \sqrt{(j \mp m)(j \pm m_1)} = \sum_{m_1, m_2} (J_{1\pm} + J_{2\pm}) |j_1 j_2; m_1 m_2\rangle (CGC), \tag{15.45}$$

where (CGC) is the Clebsch-Gordon Coeficcient, $\langle j_1 j_1 m_1 m_2 | j_1 j_2; jm\rangle$. We can rewrite the last equation as

$$\begin{aligned} &\hbar \sum_{m_1, m_2} [(j_{1\pm} |j_1 m_1\rangle \otimes |j_2 m_2\rangle) + (|j_1 m_1\rangle \otimes J_{2\pm} |j_2 m_2\rangle)] \\ &= \sum_{m_1, m_1} \Big[\sqrt{(j_1 \mp m_1)(j_1 \pm m_1 + 1)} |j_1 m_1 \pm 1\rangle \otimes |j_2 m_2\rangle + \\ &\quad + \sqrt{(j_2 \mp m_2)(j_2 \pm m_2 + 1)} |j_1 m_1\rangle \otimes |j_2 m_2 \pm 1\rangle\Big](CGC), \end{aligned} \tag{15.46}$$

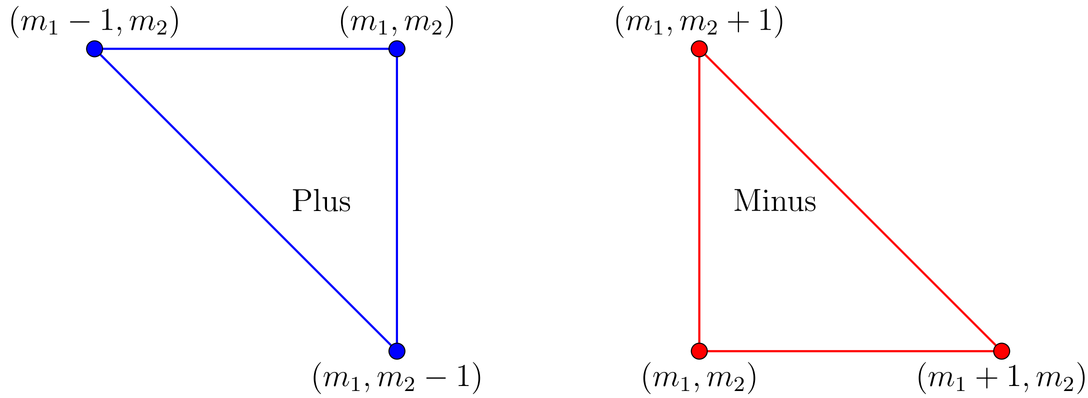

Figure 6: Visual Interpretation of Clebsch-Gordon Coefficients

Which we can set equal to

$$\hbar\sqrt{(j\mp m)(j\pm m+1)}\times\sum_{m_1'm_2'}|j_1j_2;m_1'm_2'\rangle\,\langle j_1j_1m_1'm_2'|j_1j_2;jm\rangle \tag{15.47}$$

and we can take matrix elements as

$$\begin{aligned}&\langle j_1j_2m_1'm_2'|j_1j_2;m\pm 1\rangle\,\hbar\sqrt{(j\pm m)(j\pm m+1)}\\&=\sum_{m_1,m_2}\Big[\hbar\sqrt{(j_1\mp m_1)(j_1\pm m_1+1)}\delta_{m_2',m_2}\delta_{m_1',m_1\pm1}\\&\quad+\hbar\sqrt{(j_2\mp m_2)(j_2\pm m_2+1)}\delta_{m_1,'m_2}\delta_{m_2',m_2\pm1}\Big]\,\langle j_1j_2m_1m_2|j_1j_2;jm\rangle\,,\end{aligned} \tag{15.48}$$

which leads to the recursion relation,

$$\begin{aligned}&\sqrt{(j\pm m)(j\pm m+1)}\,\langle j_1j_1;m_1'm_2'|j_1j_2;jm\pm 1\rangle\\&=\sqrt{(j_1\pm m_1')(j_1\pm m_1'+1)}\,\langle j_1j_2;m_1'\mp 1,m_1|j_1j_2;jm\rangle\\&\quad+\sqrt{(j_2\mp m_2')(j_1\pm m_2'+1)}\,\langle j_1j_2;m_1',m_1\mp 1|j_1j_2;jm\rangle\end{aligned} \tag{15.49}$$

No we will drop the primes and we will see how we can actually solve coefficients in the m_1, m_2 plane. This is shown in Figure 6 Although we can in principle calculate all of these through the recursion relation, in practice one just looks these up.

15.3.1 Wigner D-Matrices

Clebsch-Gordon Coefficients allow us to relate Wigner D-Matrices given as

$$D'_{mm'}(R)=\langle jm|D(R)|jm'\rangle\,, \tag{15.50}$$

but we also know that if we have two systems with momentum J_1, J_2, we can associate a total J with them. So whatClebsch-Gordon tells us is that

$$|jm\rangle=\sum|j_1m_1\rangle\otimes|j_1m_2\rangle\,(CGC). \tag{15.51}$$

Since we know that

$$D(R)=D^{(1)}\otimes D^{(2)}(R), \tag{15.52}$$

which allows us to write

$$D(R)\,|jm\rangle = \sum D^{(1)}(R)\,|j_1 m_1\rangle \otimes D^{(2)}(R)\,|j_2 m_2\rangle\,(CGC), \tag{15.53}$$

which allows us to apply the Clebsch-Gordon relation and we get that

$$D^{(1)}(R)\,|j_1 m_1\rangle \otimes D^{(2)}(R)\,|j_2 m_2\rangle = \sum_{jm} D(R)\,|jm\rangle\,(CGC). \tag{15.54}$$

We can now take matrix elements (or mulply both sides by $\langle j_1 m_1'| \otimes \langle j_1 m_2'|$ and we get that

$$\begin{aligned}
&\left\langle j_1 m_1'|D^{(1)}(R)|j_1 m_1\right\rangle \otimes \left\langle j_2 m_2'|D^{(2)}(R)|j_2 m_2\right\rangle \\
&= \sum_{jm} \langle j_1 j_2; m_1' m_2'|D(R)|jm\rangle \langle jm|j_1 j_2 m_1 m_2\rangle \\
&= \sum_{jmm'} \langle j_1 j_2 m_1' m_2'|j_1 j_2, jm'\rangle \underbrace{\langle jm'|D(R)|jm\rangle}_{D^{(j)}_{m'm}(R)} \langle jm|j_1 j_2 m_1 m_2\rangle\,,
\end{aligned} \tag{15.55}$$

which leads to the following relation known as a Clebsch-Gordon series

$$D^{(j_1)}_{m_1' m_1}(R) D^{(j_2)}_{m_2' m_2}(R) = \sum_{m,m'} D^{(j)}_{m'm} \langle j_1 j_2 m_1' m_2'|j_1 j_1 jm'\rangle \langle jm|j_1 j_2 m_1 m_2\rangle\,. \tag{15.56}$$

This can provide a very "sick" (as said by professor) relationship for the spherical harmonics since

$$D^{(l)}_{m0} = Y^*_{lm}(\theta, \phi). \tag{15.57}$$

We wind up getting that equation 3.8.74 in Sakurai which as general form

$$Y^{m_1 *}_{l_1} Y^{m_2 *}_{l_1} = \left(\frac{\sqrt{(2l_1+1)(2l_2+1)}}{4\pi} \right) \sum_{l'm'} (CGC)(CGC) Y^{m'}_{l'}, \tag{15.58}$$

which gives us the general form of an integral (3.8.73) which is useful for atomic physics.

16 Spherical Tensors

16.1 Cartesian Tensors

First we want to define a tensor. The most familiar form of a tensor that we know is a vector. We want to have quantum operators which are vectors and the requirement has to be the expectation values will transform under rotation as we would expect. on the other hand, we know what a rotation a rotation does to operators since

$$V_i' = D(R)^\dagger V_i D(R), \tag{16.1}$$

Where $D(R) = \exp\left(-\frac{\vec{J}\cdot\hat{n}}{\hbar}\phi\right)$. this means that for every state α,

$$\left\langle \alpha|D(R)^\dagger V_i D(R)|\alpha\right\rangle = \sum_j R_{ij} \langle \alpha|V_j|\alpha\rangle\,. \tag{16.2}$$

We are not so good at calculating exponential, so we do it by considering infinitesimals ($\phi \to \epsilon$) to get the relation

$$\left(1 + i\epsilon\frac{J\cdot\hat{n}}{\hbar}\right)V_i\left(1 - i\epsilon\frac{J\cdot\hat{n}}{\hbar}\right) = \sum_j R_{ij}(\epsilon_j\hat{n})V_j. \tag{16.3}$$

If we choose $\hat{n} = \hat{z}$, then the rotation matrix becomes

$$R(\epsilon, \hat{z}) = \begin{pmatrix} 1 & -\epsilon & 0 \\ -\epsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{16.4}$$

and so if we expand to linear order we get

$$V_i + \frac{i\epsilon}{\hbar}[J\cdot\hat{z}, V_i] = V_i + \sum_{j\neq i} R_{ij}(\epsilon)V_j = V_i + \epsilon\sum_{j\neq i}\epsilon_{ijz}V_j. \tag{16.5}$$

This implies that

$$\frac{i\epsilon}{\hbar}[J_z, V_i] = -\epsilon\sum_{j\neq i}\epsilon_{ijz}V_j, \tag{16.6}$$

and we can cancel the epsilons to get that

$$[J_z, V_i] = i\hbar\sum_j \epsilon_{ijz}V_j \tag{16.7}$$

and also

$$[V_i, J_j] = i\hbar\sum_k \epsilon_{ijk}V_k, \tag{16.8}$$

and these commutation relations define a vector operator. Now we need a definition for tensors. We will also define it by saying how it transforms under rotation. So we can write

$$T_{ijk\ldots} \to T'_{ijk\ldots} = \sum_{i'j'k'\ldots} R_{ii'}R_{jj'}\ldots T_{i'j'k'\ldots}. \tag{16.9}$$

These are called Cartesian tensors and while a perfectly valid object, they are not efficient, so we will use spherical tensors instead.

16.2 Spherical Tensor Definition

So we can use the identity

$$U_iV_j = \frac{(\vec{U}\cdot\vec{V})}{3}\delta_{ij} + \frac{U_iV_j - U_jV_i}{2} + \left(\frac{U_iV_j + U_jV_i}{2} - \frac{U\cdot V}{3}\delta_{ij}\right) \tag{16.10}$$

So we want to give a list of tensors to build up to spherical tensors. We will take our example vector to be $\vec{r}$. In Cartesian coordinates this would correspond to (x, y, z). For a rank two tensor, we have $T = \vec{r}\otimes\vec{r}$ which we are looking at because of its rotation properties. For cartesian tensors, we would have that

$$T_xx = x^2 \tag{16.11}$$

$$T_yy = y^2 \tag{16.12}$$

$$T_{xy} = xy \tag{16.13}$$

$$\vdots, \tag{16.14}$$

and they linearly rotate. Now if we look at irreducible tensors

$$r^2/3 = T_{r^2} \tag{16.15}$$

$$z^2 - \frac{r^2}{3} = T_{z^2} \tag{16.16}$$

$$x^2 - y^2 = T_{x^2-y^2} \tag{16.17}$$

$$xy = T_{xy} \tag{16.18}$$

$$yz = T_{yz} \tag{16.19}$$

$$zx = T_{zx}, \tag{16.20}$$

where the first three are decoupled under rotation from the last three. We can then define the spherical tensor

$$r^2 Y_{00}(r) = r^2 \tag{16.21}$$

$$r^2 Y_{20}(r) = \frac{3z^2 - r^2}{3} \tag{16.22}$$

$$r^2 Y_{2\pm}(r) = 2(x \pm iy)z \tag{16.23}$$

$$r^2 Y_{2\pm 2}(r) = (x \pm iy)^2, \tag{16.24}$$

where we have dropped some prefactors. These are also irreducible.

16.3 Rotations of Spherical Harmonics

We use the spherical tensors $T_{kq}(\vec{V}) = |V|^k Y_{l=k,m=q}\hat{V}$ since we can figure out the rotations by wigner-d matrices in a somewhat straightforward manner. So we can look at

$$\begin{aligned} Y_{lm}(R\hat{V}) &\propto T_{kq}(R\vec{V}) \\ &= \left\langle R\hat{V})|lm\right\rangle = \left\langle \hat{V}|D(R)^\dagger|lm\right\rangle \\ &= \sum_{l',m'} \left\langle \hat{V}|l'm'\right\rangle \underbrace{\langle lm|D(R)|l'm'\rangle^*}_{\delta_{l,l'} D^{(l)*}_{m,m'}} \\ &= \sum_{m'} Y_{lm'}(\hat{V}) D^{(l)}_{m,m'}(R)^* \end{aligned} \tag{16.25}$$

Thi leads us to

$$T_{k=l,q-m}(R\hat{V}) = \sum_{m'} T_{k,q=m'}(\hat{V} D^{(l)}_{mm'}(R)^*, \tag{16.26}$$

which implies that

$$D(r)^\dagger T^{(k)}_q D(R) = \sum_{q'} D^{(k)}_{q,q'}(R)^* T^{(k)}_{q'}, \tag{16.27}$$

and so anything satisfying this relation is a spherical tensor. The motivation is that things that rotate like spherical harmonics are spherical tensors. In order for this to be useful, we need a way of calculating the wigner D matrices. The way in which we will do this (although one could in principle calculate the full matrices in mathematica) is to look at infinetesimal rotations. So we use again

$$D(R) = \left(1 - i\frac{\vec{j}\cdot\hat{n}}{\hbar}\phi\right), \tag{16.28}$$

which if we plug into the equation gives us

$$T_q^{(k)} - \frac{i\phi}{\hbar}[\vec{J}\cdot\hat{n}, T_q^{(k)}] = \sum_q{}' T_{q'}^{(k)} \left\langle kq \left| \left(1 - i\frac{\vec{j}\cdot\hat{n}}{\hbar}\phi\right) \right| kq' \right\rangle^* , \tag{16.29}$$

which we can reduce to

$$[\vec{J}\cdot\hat{n}, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)} \left\langle kq|\vec{J}\cdot\hat{n}|kq'\right\rangle . \tag{16.30}$$

So if we choose $\hat{n} = \hat{z}$, then we get that

$$[J_z, T_q^{(k)}] = \hbar q T_q^{(k)}. \tag{16.31}$$

If we choose $\hat{n} = \hat{x} \pm i\hat{y}$, we gt that

$$[J_\pm, T_q^{(k)}] = \hbar\sqrt{(k\mp q)(k\pm q+1)}T_{q\pm 1}^{(k)}. \tag{16.32}$$

This will be the working definition for the spherical tensors.

16.4 Construction of Sherical Tensors

For scalars, rank 0 tensors, and vectors, rank 1 tensors, we have plenty of experience with manipulation and construction. The important result is that products of spherical tensors give higher rank tensors. So the big theorem is that

$$\sum_{q_1,q_1} X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} \left\langle k_1, k_1, q_1, q_2 | k_1 k_2; k_q \right\rangle = T_q^{(q)}, \tag{16.33}$$

where

$$|k_1 - k_2| \leq k \leq k_1 + k_2, \tag{16.34}$$

which comes from the properties of the Clebsch-Gordon coefficients. So if we combine two vectors U and V, we get a sum of spherical tensors of rank 0,1,2. The proof of this is long and very algebraic.

16.5 Wigner-Eckart Theorem

Now we give the Wigner-Eckart theorem which is the motivation behind most of this. It will allow us to more easily calculate matrix elements. It tells us we can compute

$$\left\langle \alpha, j', m' | T_q^{(k)} | \alpha, j, m \right\rangle = \left\langle jk; j'm' | kj; qm \right\rangle \frac{\left\langle \alpha' j' || T^{(k)} || \alpha j \right\rangle}{\sqrt{(2j+1)}}, \tag{16.35}$$

which is just a Clebsch-Gordon coefficient times stuff that does not depend on q or m. Practically speaking it allows us to only have to calculate this stuff once and then use it to get everything else. The stuff is essentially a proportionality constant to the Clebsch-Gordon coefficient.