# 1 Lecture 1 (Mar. 5th)

**Chapter 1** The Emergence of Quantum Physics

**Theorem.** (A free particle as a plane wave) It was De Broglie that first suggested that all particles have wave-like properties and that equations for light can also be used to describe arbitrary particles

$$(E/c, p) = \hbar(\omega/c, k)$$

As such, we will model a free particle with a precise momentum can as a complex plane wave.

$$\psi(x,t) = A \exp i\Big(\frac{px}{\hbar} - \frac{Et}{\hbar}\Big)$$

Notice how the group velocity ($d\omega/dk$) is precisely the velocity of the particle as expected.

**Definition.** (Schrodinger's equation) Differentiating,

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi \qquad -i\hbar\frac{\partial\psi}{\partial x} = p\psi$$

Consider spliting the wave functions into two parts each dependent on $x$ and $t$

$$\psi(x,t) = \exp\Big(\frac{-iEt}{\hbar}\Big)\psi(x)$$

with $\psi(x) = \exp\{ipx/\hbar\}$. In non-relativistic cases of free particles, energy is expressed as

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

Attempting to obtain the form of this energy,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = \frac{p^2}{2m}\psi = E\psi$$

The following equation is called the Schrodinger equation. Furthermore, we know that with scalar potential energy $V$, energy is expressed as $E = p^2/2m + V$. Then by extension we have

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

which is called the time-independent Schrodinger equation. When we consider time-dependence, we have $E\psi(x)$ expressed as a derivation, or

$$\Big(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\Big)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

## 2 Lecture 2 (March 10th)

**Proposition.** (Born Interpretation) In 1926, Born noticed that the Schrodinger equation must mathematically contain a radiation element, and proposed that it had to show the probability of the particle. The wave function being a complex function, it is natural to interpret its squared norm as probability, with

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

for all time $t$ and the integral being evaluated over all space. The important part is for the integral to be finite, or in other words, square integrable.

**Theorem.** (Expectation of an observable quantity with zero standard deviation ) Recall that expectation $\langle A \rangle = a$ (observable with real expectation) for $0 \leq P_n \leq 1$ and $\sum_n P_n = 1$ is given by

$$\langle A \rangle = \sum_n A_n P_n \to \int_{-\infty}^{\infty} dx \, |\psi(x)|^2 A(x) \to \int_{-\infty}^{\infty} dx \, \psi^*(x) \Big( A(x)\psi(x) \Big)$$

The right handside is a parallel statement written in operator notation. An important point is that when the expectation value converges to a singular value $\langle A \rangle = a$, we expect to have a negligible variance (standard deviation$^2$) which we can mathematically express as

$$\langle (A-a)^2 \rangle = \int_{-\infty}^{\infty} \psi^*(A-a)^2\psi = \int_{-\infty}^{\infty} \psi^*(A-a)\Big[(A-a)\psi\Big] = \int_{-\infty}^{\infty} \Big[(A-a)\psi\Big]^* \Big[(A-a)\psi\Big]$$

If we were to take $A$ as an operator on $\psi$, the last equality would be only true when we impose that the operator $A$ is Hermitian which we will study later on. The above can be further simplified as

$$\int_{-\infty}^{\infty} |(A-a)\psi|^2 \geq 0$$

For the above to be zero, we must have $A\psi = a\psi$. In a general setting, we will show that, given that $A$ is a Hermitian operator, $A$'s expectation values will be seen as the eigenvalues of the operator.

**Theorem.** (Shared eigenstates imply commutative operators) Suppose that two operators share eigenstates, that is, they share states in which their standard deviations are zero.

$$A(B\psi) = A(b\psi) = ba\psi = ab\psi = B(a\psi) = B(A\psi)$$

The above shows how $(AB - BA)\psi = 0$ and $[A, B] = 0$ (the two operators commute). This implies that for non-commuting operators ($[\hat{x}, \hat{p}] = i\hbar$), their eigenstates necessarily cannot be identical and that expectation values have non-zero variance ($\varDelta x \varDelta p \geq i\hbar$).

## 3 Lecture 3 (March 12th)

**Chapter 2** Wave Particle Duality, Probability, and the Schrodinger Equation

**Definition.** A vector space $V$ is defined as an abelian group with respect to addition with scalar multiplication

**Example.** All square integrable functions defined on an interval $L^2(I)$ forms a vector space

$$\int_I |\psi|^2 < \infty$$

**Theorem.** (Wave packets) We have studied the following form of a plane wave as an ansatz for our wave function

$$e^{i(kx-\omega(k)t)}$$

where $k \to p/\hbar$ and $\omega \to E/\hbar$. Consider a wave packet out of a superposition of waves with weight $A(k)$.

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, A(k) e^{i(kx-\omega(k)t)}$$

Notice that the frequency of the wave is given by the dispertion relation $\omega(k)$. When $t = 0$,

$$\psi(x,0) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, A(k) e^{ikx}$$

with the weight function (Fourier transform) given by

$$A(k) = \int_{-\infty}^{\infty} dx\ \psi(x,0) e^{-ikx}$$

**Theorem.** Define $y = ax$ and $x = y/a$

$$\int dx\ \delta(x) = 1 = \int dy\ \delta(y) = |a| \int dx\ \delta(ax)$$

we then have

$$\delta(ax) = \frac{1}{|a|}\delta(x)$$

On the other hand,

$$\begin{aligned}\delta(x^2 - a^2) =& \delta((x+a)(x-a)) \\ =& \frac{1}{2|a|}\delta(x-a) + \frac{1}{2|a|}\delta(x+a)\end{aligned}$$

and more generally,

$$\delta(f(x)) = \sum_i \delta((x - x_i) f'(x_i)) = \sum_i \frac{1}{|f'(x_i)|} \delta(x - x_i)$$

## 4 Lecture 4 (March 17th)

**Remark.** The metric $d : V \times V \to \boldsymbol{R}$ in the $L^2$ space is defined as

$$d(f, g) = \sqrt{\int_I |f - g|^2} \geq 0$$

We have previously made the remark that

$$d(f, g) = 0 \iff [f] = [g]$$

We note that the metric satisfies the triangle inequality,

$$d(f, g) \leq d(f, h) + d(h, g)$$

Which completes our proof that the function is indeed a metric.

**Definition.** A Cauchy sequence is a sequence $\{x_n\}$ such that for all $\varepsilon > 0$ there exists a $N$ such that for all $m, n > N$,

$$d(x_n, x_m) < \varepsilon$$

**Definition.** A set is called complete if all Cauchy sequences in the set converge to a element in the set.

$$\lim_{n \to \infty} x_n = x \in V$$

It is important to note that $L^2(I)$ is complete (Riesz-Fisher theorem).

**Theorem.** (Uncertainty principle seen as the product of distribution deviations) We have previously shown that a wave function can be expressed as

$$\Psi(x, t) = \int \frac{dk}{2\pi} A(k) \exp(ikx - i\omega(k)t)$$

Assume that the distribution of $A(k)$ is given as

$$A(k) = \exp\Big[ - \frac{(k - k_0)^2}{\alpha} \Big]$$

Then the approximate width (the distance between the maximum of the distribution and the point where the graph falls to $1/e$) would be given as $(\Delta k/2)^2 = \alpha$ and $\Delta k = 2\sqrt{\alpha}$.

Integrating the function at $t = 0$,

$$\begin{aligned}\psi(x,0) &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\Big[-\frac{(k-k_0)^2}{\alpha} + ikx\Big] \\ &= \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \exp\Big[-\frac{k'^2}{\alpha} + i(k_0+k')x\Big] \\ &= \exp(ik_0x) \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \exp\Big[-\frac{k'^2}{\alpha} + ik'x\Big] \\ &= \exp\Big(ik_0x - \frac{\alpha x^2}{4}\Big) \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \exp\Big[-\frac{1}{\alpha}\Big(k' - \frac{i\alpha x}{2}\Big)^2\Big]\end{aligned}$$

with $k' = k - k_0$ leading to $k = k' + k_0$. Recall that for $a \in \boldsymbol{R} > 0$,

$$\int_{-\infty}^{\infty} e^{-ax^2} = \sqrt{\frac{\pi}{a}}$$

However, the integral above can be done on a closed contour $\mathcal{C}$. Cauchy's theorem states that on this contour,

$$\oint_{\mathcal{C}} dz\ f(z) = 0$$

if $f(z)$ is analytic. An example of such a function $e^{-z^2}$. With this knowledge, we preform the integral without the imaginary part shift along the real axis from $+\infty$ to $-\infty$ and down to $y = q - i\alpha x/2$ and back to positive infinity.

$$\oint_C dk'\ f(k') = 0 = (\text{wanted}) - \exp\Big[ik_0x - \frac{\alpha x^2}{4}\Big] \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \exp\Big[-\frac{k'^2}{\alpha}\Big]$$

which results in

$$(\text{wanted}) = \exp\Big[ik_0x - \frac{\alpha x^2}{4}\Big] \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \exp\Big[-\frac{k'^2}{\alpha}\Big] = \exp\Big[ik_0x - \frac{\alpha x^2}{4}\Big] \frac{1}{2}\sqrt{\frac{\alpha}{\pi}}$$

In sum,

$$\Psi(x,0) = \frac{1}{2}\sqrt{\frac{\alpha}{\pi}} \exp\Big[ik_0x - \frac{\alpha x^2}{4}\Big]$$

Preforming the operation to find the width again, we find $\Delta x = 4/\sqrt{\alpha}$ and thus $\Delta k \Delta x = 8$, a single number.

**Theorem.** (The group velocity of the wave packet as the velocity of the particle) What about the case where the wave function evolves throughout time?

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\ A(k) e^{ikx - i\omega(k)t}$$

Preforming a Taylor expansion about $k_0$,

$$\omega(k) = \omega(k_0) + \Big(\frac{d\omega}{dk}\Big)_{k=k_0}(k-k_0) + \frac{1}{2}\Big(\frac{d^2\omega}{dk^2}\Big)_{k=k_0}(k-k_0)^2 + \dots$$

Here, we can substitute $(d\omega/dk)_{k=k_0} = v_g$ and $(k-k_0) = q$. Ignoring the higher order terms, we have for the wave function

$$\psi(x,t) = e^{i(k_0 x - \omega(k_0)t)} \int_{-\infty}^{\infty} \frac{dq}{2\pi}\, A(q+k_0) e^{iq(x-v_g t)} \exp\Big[-\frac{iq^2 t}{2}\Big(\frac{\partial^2\omega}{\partial k^2}\Big)_{k=k_0}\Big]$$

We realise that we can preform the integral alike the one we did beforehand and results in (with the substitution of $\beta$ for the second derivative),

$$\psi(x,t) = \sqrt{\frac{2\pi}{\alpha + i\beta t}} \exp\Big[ik_0 x - i\omega(k_0)t - \frac{1}{2}\frac{(x-v_g t)^2}{\alpha + i\beta t}\Big]$$

The result's main punchline is that the wave has a maximum when $x - v_g t = 0$. That is, the wave-particle has the group velocity of the wave! ($v_g|_{\text{wave}} \iff v|_{\text{particle}}$)! The probability $|\psi(x,t)|^2$ becomes

$$\frac{2\pi}{\sqrt{\alpha^2 + \beta^2 t^2}} \exp\Big\{-\frac{\alpha(x-v_g t)^2}{\alpha^2 + \beta^2 t^2}\Big\}$$

The width for this is $2\sqrt{(\alpha^2 + \beta^2 t^2)/\alpha}$, which poses a problem. Despite this, $\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2$ is a constant independent of time, which alleviates the problem theoretically.

$$\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 = 2\pi\sqrt{\frac{\pi}{\alpha}}$$

## 5 Lecture 5 (March 19th)

**Theorem.** (Explaination of the collapse of the wave function) Consider the double slit experiment with electrons. The electron going through the first slit would be expressed as $\psi_1$ and the electron going through the second slit would be expressed as $\psi_2$. The resulting distribution on the screen would be expressed as

$$|\psi_1 + \psi_2|^2$$

giving an interference pattern. However, if we were to disturb the first slit's wave with photons used for observation, we could achieve

$$\begin{aligned}|e^{i\phi_1}\psi_1+\psi_2|^2 =&(e^{i\phi}\psi_1+\psi_2)(e^{-i\phi}\psi_1^*+\psi_2^*)\Big|_{\text{avg}}\\ =&|\psi_1|^2+|\psi_2|^2+e^{-i\phi}\psi_1^*\psi_2+e^{i\phi}\psi_1\psi_2^*\Big|_{\text{avg}}\\ =&|\psi_1|^2+|\psi_2|^2\end{aligned}$$

as $\langle\cos\phi\pm i\sin\phi\rangle_{\text{avg}}=0$. This is the result we actually see experimentally, with two Gaussian distributions.

**Definition.** (Wave packets) We have previously learned the wave packet description

$$\Psi(x,t)=\int\frac{dp}{\sqrt{2\pi\hbar}}\phi(p)\exp\Big(\frac{ipx}{\hbar}-\frac{iE(p)t}{\hbar}\Big)$$

The idea by De Broglie to apply the logic of waves to particles was revolutionary. At $t=0$, the energy term disappears, resulting in

$$\Psi(x,t=0)=\int\frac{dp}{\sqrt{2\pi\hbar}}\phi(p)\exp\Big(\frac{ipx}{\hbar}\Big)\longleftrightarrow\phi(p)=\int\frac{dx}{\sqrt{2\pi\hbar}}\Psi(x,t=0)\exp\Big(\frac{-ipx}{\hbar}\Big)$$

In this way, we see two different wavefunctions (each in the position space and momentum space space) which give equivalent physical information.

Previously, we have found that the plane wave equation, that models a free particle with definite momentum and indefinite position, follows the Schrodinger equation. We now look for the differential equation in the quantum landscape.

**Definition.** (Schrodinger Equation) We have verified that complex plane waves satisfy the Schrodinger equation. We now verify that wave packets do also.

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\int\frac{dp}{\sqrt{2\pi\hbar}}\phi(p)E(p)\exp\Big(\frac{ipx}{\hbar}-\frac{iE(p)t}{\hbar}\Big)$$

and

$$\frac{1}{2m}\Big(-i\hbar\frac{\partial}{\partial x}\Big)^2\Psi(x,t)=\int\frac{dp}{\sqrt{2\pi\hbar}}\phi(p)\frac{p^2}{2m}\exp\Big(\frac{ipx}{\hbar}-\frac{iE(p)t}{\hbar}\Big)$$

(We can of course extend our definition to multiple dimensions and we would have $\partial^2/\partial x^2\to\nabla^2$) If there exists potential, we can simply add $V(x)$ to the differential operator, giving

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

for a free particle. What we have obtained is the time dependent Schrodinger equation.

**Remark.** (Boundary condition for normalisation and the probability current) Let's do a very important calculation! As we mentioned that the wave function denotes probability, we require that the wave functions are normalized, that is,

$$\int dx\, |\Psi(x,t)|^2 = 1$$

for all time t. Note that $\int dx\, |\Psi(x,t=0)|^2 = 1$ is rather simple to normalise, but the tricky part is when $t > 0$, where the result might be a function of $t$. In a more formally manner, we ask: does time evolution preserves total probability? The answer lies in the Schrodinger equation, whose left-hand-side generates time evolution. We impose the following boundary condition:

$$\frac{\hbar}{2im}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \frac{\partial\Psi}{\partial x}\Psi^*\right)\Big|_a^b$$

*Proof.* Note that

$$\begin{cases} \left(-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V(x)\right)\Psi = i\hbar\dfrac{\partial\Psi}{\partial t} \\ \left(-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V(x)\right)\Psi^* = -i\hbar\dfrac{\partial\Psi^*}{\partial t} \end{cases}$$

We then have

$$\begin{aligned} 0 &= \frac{d}{dt}\int_a^b dx\,\Psi\cdot\Psi^* = \int_a^b dx\left(\frac{\partial\Psi}{\partial t}\Psi^* + \Psi\frac{\partial\Psi^*}{\partial t}\right) \\ &= \int_a^b \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}\right)\Psi^*\,dx + \frac{1}{i\hbar}\left(\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\right)\Psi\,dx \\ &= \int_a^b dx\,\frac{\hbar}{2im}\frac{\partial}{\partial x}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \frac{\partial\Psi}{\partial x}\Psi^*\right) = \frac{\hbar}{2im}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \frac{\partial\Psi}{\partial x}\Psi^*\right)\Big|_a^b \\ &= -j(x,t)\Big|_a^b \end{aligned}$$

From here, we impose that the last term is equal to zero, which allows the probability interpretation to be valid. This is a boundary condition for the wavefunction to follow. In multiple dimensions,

$$\int_V d\mathbf{x}\,\frac{\hbar}{2im}\nabla\cdot[(\nabla\Psi^*)\Psi - \Psi^*(\nabla\Psi)]$$

and using Stoke's law, we change the requirement to

$$-\frac{\hbar}{2im}\int \mathbf{j}(x,t)\cdot d\mathbf{a} = 0$$

□

## 6 Lecture 6 (March 24th)

**Recall.** We have previously investigated a condition for which the probabilistic interpretation for quantum mechanics was valid.

$$0 = \frac{d}{dx}\int dx\, \Psi^*\Psi = \int dx\, \frac{\partial}{\partial t}(\Psi^*\Psi) = -\int dx\, \frac{\partial}{\partial x} j(x,t)$$

Where

$$j(x,t) = \frac{\hbar}{2im}\Big(\frac{\partial \Psi}{\partial x}\Psi^* - \Psi\frac{\partial \Psi^*}{\partial x}\Big)$$

is called the probability current density. We can see how the above formulation states that

$$-\oint dA\, \mathbf{n}\cdot\mathbf{j}(x,t) = 0$$

For the above to work, we require that the current density satisfies

$$\frac{\partial}{\partial t}(\Psi^*\Psi) + \nabla\cdot\mathbf{j}(x,t) = 0$$

which is analogous to the continuity equation with $\rho = \Psi^*\Psi$ and $\mathbf{j}(x,t) = \mathbf{J}(x,t)$.

**Example.** We see that for the following wave function, our idea that current density is equal to density times velocity aligns with our definition.

$$\psi(x) = C\exp\left(i\frac{px}{\hbar}\right)$$

we find the probability density to be $c^2p/m$ which exactly $(\psi\psi^*)v = \rho v$. This makes sense as this is exactly density times what we expect to be velocity.

**Remark.** (Expectation value) In quantum mechanics, we seek the expectation value of a measurable quantity $f(x)$. Given a probability wave $\Psi(x,t)$, we have

$$\langle f(x)\rangle = \int dx\ \Psi^*(x,t)f(x)\Psi(x,t)$$

we notice that as wave functions are dependent of time, the expectation values also have a time dependence. Let's verify that $\langle p\rangle = md/dt\langle x\rangle$ with $p \to -i\hbar\partial/\partial x$

$$\begin{aligned}\langle p\rangle =& m\frac{d}{dt}\langle x\rangle\\ =& \int dx\ \Psi^*(x,t)x\Psi(x,t)\\ =& m\frac{\hbar}{2i}\int dx\ \Big(\underbrace{\Big(\frac{\partial^2}{\partial x^2}\Psi^*\Big)x\Psi}_{\dagger} - \Psi^*x\frac{\partial^2}{\partial x^2}\Psi\Big)\end{aligned}$$

Using Schrodinger's equation. Then,

$$\begin{aligned}
\dagger =& \frac{\partial}{\partial x}\Big(\frac{\partial \Psi^*}{\partial x} x\Psi\Big) - \frac{\partial \Psi^*}{\partial x}\frac{\partial}{\partial x}(x\Psi) \\
=& \frac{\partial}{\partial x}\Big(\frac{\partial \Psi^*}{\partial x} x\Psi\Big) - \frac{\partial}{\partial x}\Big(\Psi^* \frac{\partial}{\partial x}(x\Psi)\Big) + \Psi^* \frac{\partial^2}{\partial x^2}(x\Psi)
\end{aligned}$$

However, the last term becomes (as $(fg)'' = f'' + 2f'g' + g''$)

$$\Psi^*\Big(2\frac{\partial \Psi}{\partial x} + x\frac{\partial^2 \Psi}{\partial x^2}\Big)$$

Altogether,

$$\langle p \rangle = (\text{boundary}) + (-i\hbar)\int dx\ \Psi^* \frac{d}{dx}\Psi$$

We now ask: is there no problem when the observable is a polynomial expression of $x$ and $p$? See that

$$\begin{aligned}
\hat{x}\hat{p}\Psi(x) =& \hat{x}(-i\hbar\frac{\partial \Psi}{\partial x}) \\
=& x(-i\hbar\frac{\partial \Psi}{\partial x}) \\
\hat{p}\hat{x}\Psi =& (-i\hbar)\frac{\partial}{\partial x}(\hat{x}\Psi) \\
=& (-i\hbar)(\Psi + x\frac{\partial \Psi}{\partial x})
\end{aligned}$$

We thus see that

$$(\hat{x}\hat{p} - \hat{p}\hat{x}) = [\hat{x}\hat{p} - \hat{p}\hat{x}] = i\hbar$$

This is called the fundamental canonical commutator relation. We find that we should be careful with the order in which $\hat{x}$ and $\hat{p}$ is applied ($\hat{x}^2\hat{p}^2 \neq \hat{x}\hat{p}^2\hat{x}$).

**Remark.** We emphasize that $\hat{A}$ must have a real expectation value given by

$$\langle \hat{A} \rangle = \int \Psi^* \hat{A} \Psi$$

Or equivalently, $\hat{A}$ is Hermitian. We see that, indeed, for the momentum operator,

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

and that

$$\langle p \rangle^* - \langle p \rangle = i\hbar \int dx\ \frac{\partial}{\partial x}(\Psi^*\Psi) = i\hbar \Psi^*\Psi\Big|_{-\infty}^{\infty} = 0$$

In a similar manner, we can see that all polynomial expressions of $\hat{x}$ and $\hat{p}$ are Hermitian, and that the Hamiltonian operator also is. With the definition of the Hamiltonian operator, we can write the Schrodinger equation as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t)$$

**Remark.** Let's see that the wave-packet in the momentum space can be normalized.

$$\begin{aligned}
1 = \int_{-\infty}^{\infty} dx\ |\Psi(x)|^2 &= \int_{-\infty}^{\infty} dx\ \Psi^*(x)\Psi(x) \\
&= \int dx \int \frac{dp'}{\sqrt{2\pi\hbar}} \int \frac{dp}{\sqrt{2\pi\hbar}} \phi^*(p')\phi(p) \exp\left\{\frac{-ip'x + ipx}{\hbar}\right\} \\
&= \int dp\ |\phi(p)|^2
\end{aligned}$$

From the fact that the integral of the exponential term is $2\pi\hbar\delta(p-p')$. What have we learned? We have obtained the Parseval relation that tells us that if the wave function in the position space is squared-integrable, the function in the momentum space also is.
We can also ask, then, what the momentum operator is in the momentum space.

$$\langle\hat{p}\rangle = \int \Psi^*(x)(-i\hbar)\frac{\partial\Psi}{\partial x} = \int \frac{dp'}{\sqrt{2\pi\hbar}} \exp\left\{\frac{-ip'x}{\hbar}\right\}\phi^*(p')\Big(-i\hbar\frac{\partial}{\partial x}\Big)\int \frac{dp}{\sqrt{2\pi\hbar}} \exp\left\{\frac{ipx}{\hbar}\right\}\phi(p)$$

which becomes

$$\int dp\ \phi^*(p)p\phi(p)$$

## 7 Lecture 7 (March 26th)

**Remark.** We have previously learned the Heisenberg uncertainty principle, expressible as

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

This is called Heisenberg-Weyl algebra. The commutator satisfies the first Bianchi identity. By mathematical induction, we can quite easily find that

$$[x,p^n] = ni\hbar p^{n-1}$$

**Recall.** We have seen how the expected value for the momentum operator was

$$\langle\hat{p}\rangle = \int dp\ \phi^*(p)p\phi(p)$$

What would happen if we would try to find the expected value of the position using the momentum wave function?

$$\begin{aligned}
\langle \hat{x} \rangle =& \int dx\ \Psi^*(x) x \Psi(x) \\
=& \int dx\ \Big( \int \frac{dp'}{\sqrt{2\pi\hbar}} \phi^*(p) \exp\Big( -\frac{ipi'x}{\hbar}\Big)\Big) x \Big( \int \frac{dp}{\sqrt{2\pi\hbar}} \phi(p) \exp\Big(\frac{ipx}{\hbar}\Big)\Big) \\
=& -i\hbar \int dp\ dp'\ \phi^*(p')\phi(p) \Big(\frac{\partial}{\partial p}\delta(p-p')\Big) \\
=& -i\hbar \int dp'\ \phi^*(p)\phi(p)\delta(p-p')\big|_{-\infty}^{\infty} + i\hbar \int dp'\ dp\ \phi^*(p) \frac{\partial}{\partial p}(\phi(p)\delta(p-p')) = \quad \int dp\ \phi^*(p) \Big[ i\hbar \frac{\partial}{\partial p}\Big] \phi(p)
\end{aligned}$$

as

$$\int dx\ x \exp\Big(\frac{i(p-p')x}{\hbar}\Big) = -i\hbar \frac{\partial}{\partial p} \int dx\ \exp\Big(\frac{i(p-p')x}{\hbar}\Big) = -i\hbar \frac{\partial}{\partial p}(2\pi\hbar\delta(p-p'))$$

**Definition.** The basis of a vector space ($V$) is defined as a linearly independent and spanning subset of $V$. By spanning, we mean that an arbitrary vector can be expressed as a linear combination of the subset.

$$v = \sum_n c_n v_n$$

By linearly independent, we mean that if

$$\sum_n c_n v_n = 0$$

this implies $c_n = 0$ for all $n$. By a finite dimensional vector space, we mean that the number of elements in a basis is finite. Meanwhile, an inner product of a complex vector space $V$ is a machine that takes in two vectors to create a scalar. There are multiple notations you can use for this inner product ($\langle v, w\rangle$ or $(v, w)$ to name a few). We require that the map satisfies

(i) $\langle v, v\rangle \geq 0$ and $\langle v, v\rangle = 0$ if and only if $v = 0$ (non-degeneracy)

(ii) $\langle v, a_1 w_1 + a_2 w_2\rangle = a_1\langle v, w_1\rangle + a_2\langle v, w_2\rangle$ (linearity in the second argument)

(iii) $\langle v, w\rangle^* = \langle w|v\rangle$ (conjugate symmetry)

**Example.** An example is the $n$-dimensional complex space $\boldsymbol{C}^n$. An inner product of two vectors $v = (v_1, \ldots, v_n)$ and $w = (w_1, \ldots, w_n)$ is

$$\langle w, v\rangle = \sum_{i=1}^n w_i^* v_i$$

This is called the standard inner product.

**Example.** The $L^2(I)$ space is a space with square integrable functions on $I$ ($\int_I |f|^2 < \infty$).

The inner product of two vectors $f$ and $g$ is

$$\langle f, g\rangle = \int_I dx\ f^* g$$

This is an important inner product used for wave functions.

**Example.** The space of $n \times n$ complex matrices $M_{n\times n}(\boldsymbol{C})$ has the following inner product.

$$\langle M_1, M_2\rangle = \mathrm{Tr}(M_1^\dagger M_2)$$

**Definition.** A linear operator (or transformation) is a map $L : V \to W$ which satisfies

$$L(a_1 v_1 + a_2 v_2) = a_1 L(v_1) + a_2 L(v_2)$$

Some examples are matrix multiplication, scalar multiplication, and derivation. Along this line, the Hermitian operator $\hat{H}$ is a linear operator. The reason why we want linear transformations is because it preserves superposition. If the input if a superposed state, the output is likewise.

**Remark.** We can represent any linear operator as a matrix (which is called the matrix representation of the operator). For simplicity, assume a finite dimensional vector space and we have

$$L(v = \sum_{i=1}^{n} c_i v_i) = \sum_{i=1}^{n} c_i L(v_i)$$

For a single component $v_i$, we have

$$L(v_i) = \sum_{j=1}^{m} w_j L_{ji}$$

be aware of the order of the $j$ and $i$ for the matrix $L$.

## 8 Lecture 8 (March 31st)

**Recall.** The time independent Schrodinger equation was given by

$$E\psi(x) = \hat{H}\psi(x)$$

In this manner, we can take $E$ as an eigenvalue for the operator $\hat{H}$.

**Example.** We can consider the infinite potential well, where

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

The Schrodinger equation becomes

$$\Big(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\Big)\psi(x)=E\psi$$

Due to the infinities, we require that the wave function degenerates at the endpoints and beyond along with continuity. Imposing the boundary conditions, we obtain

$$\psi(x)=\sqrt{\frac{2}{a}}\sin\Big(\frac{n\pi x}{a}\Big)$$

for $n \in \boldsymbol{N}$. We then have

$$E_n=\frac{\hbar^2}{2m}\Big(\frac{n\pi}{a}\Big)^2$$

as discrete eigenvalues. Note that the functions are mutually orthogonal. We can then express an arbitrary wave function with multiple energy states as a linear combination of these values.

$$\psi(x)=\sum_n c_n\psi_n$$

Imposing the Born interpretation of quantum mechanics,

$$1=\int\psi^*\psi=\sum_{n,m}c_m^*c_n\int\psi_m^*\psi_n=\sum_n|c_n|^2$$

If we ask whether any function on the well can written as the basis above, we confront the problem that $L^2$ spaces are of infinite dimension. However, in this case, Fourier already discovered that cosine and sine functions space any function space, and we know that the set of basis functions are complete.

**Remark.** In the above, example, we saw how solving the time independent Schrodinger equation is equivalent to an eigenvalue problem, with certain wave functions forming a basis of the solution space. What about general potential? As the Hamiltonian operator is a self-adjoint differential operator, according to the Strum-Liouville theorem, eigenfunction do indeed form a basis for the solution space. Note that for Hermitian operators,

(i) Eigenvalues are real

(ii) Eigenfunctions are orthogonal

(iii) The vector space spanned by the eigenfunctions are complete

We could've also asked why the ground state of the solution space ($n=1$) is non-degenerate. The answer lies in Heisenberg's uncertainty principle.

## 9 Lecture 9 (April 2nd)

**Definition.** A parity transformation is defined as the exchange of sign of the coordinate (in three dimensions it is called inversion). In one dimension, we have

$$(\hat{P}\psi)(x) = \psi(-x) \qquad \hat{P}^2\psi = \psi$$

Considering the above as a eigenvalue problem, we have the eigenvalues $\lambda^2 = 1$. Therefore, we have even and odd functions as eigenfunctions. We now have two operators and two corresponding eigenvalues,

$$\begin{cases} \hat{P}\psi_n = (-1)^{n+1}\psi_n \\ \hat{H}\psi_n = E_n\psi_n \end{cases}$$

As the wavefunctions are simutaneously satisfy the eigenfunctions of $\hat{H}$ and $\hat{P}$, we now derive that $[H, P] = 0$.

$$\begin{aligned} (\hat{H}\hat{P})\psi(x) =& \hat{H}(\hat{P}\psi(x)) = \hat{H}(\psi(-x)) \\ \hat{P}(\hat{H}\psi(x)) =& \hat{P}\Big(-\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x)\Big) = \hat{H}\psi(-x) \end{aligned}$$

What about $\hat{P}$ and $\hat{p} = -i\hbar\, d/dx$?

$$\begin{aligned} \hat{P}(\hat{p}\psi(x)) =& \hat{P}\Big(-i\hbar\frac{d\psi(x)}{dx}\Big) = -\hbar\frac{d\psi(-x)}{d(-x)} \\ \hat{p}(\hat{P}\psi(x)) =& \hat{p}(\psi(-x)) = -i\hbar\frac{d}{dx}\psi(-x) \end{aligned}$$

We further note that $[x_i, x_j] = 0$ and that $[x_a, p_b] = i\hbar\delta_{ab}$.

**Theorem.** For an Hermitian matrix $A$, we claim that $A$'s eigenfunctions form an orthonormal basis (with real eigenvalues). An arbitrary wave function would then be expressed as

$$\psi(x) = \sum_n c_n\psi_n(x)$$

We do require that

$$\int |\psi|^2 = 1 = \sum_n |c_n|^2$$

The QM postulate is that $|c_n|^2$ is the probability that the eigenvalue $A_n$ would occur. If the operators $A$ and $B$ commute, the eigenvalues would be shared and the same eigenvector would come out.

**Example.** For the momentum operator, we have the solution

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

Calculating the inner product between two wave functions we have

$$\langle \psi_{p'} \mid \psi_p \rangle = \int_{-\infty}^{\infty} dx \ \psi_{p'}^*(x)\psi_p(x) = \int_{-\infty}^{\infty} dx \ \exp\Big(\frac{i(p-p')x}{\hbar}\Big) = \delta(p-p')$$

Let's now impose a periodic boundary condition, or $\psi_p(x) = \psi_p(x+L)$, we have

$$\exp\Big(\frac{ipL}{\hbar}\Big) = 1 \quad \to \quad p_n = \Big(\frac{2\pi}{L}\Big)n\hbar$$

for $n \in \boldsymbol{Z}$. We then have, for $p = p'$,

$$\langle \psi_{p'} \mid \psi_p \rangle = L|c|^2 = 1$$

and obtain the condition $|c| = 1/\sqrt{L}$. This process involving the boundary condition is called box quantisation.

**Example.** For a wave function given a cyclic boundary condition $\phi(x) = \phi(x+L)$ on $[-L/2, L/2]$, the Fourier expansion is given by

$$\psi(x) = \sum_{n\in\boldsymbol{Z}} A_n \exp\Big(\frac{i2\pi nx}{L}\Big)$$

with coefficients

$$A_m = \frac{1}{L}\int_{-L/2}^{L/2} dx \ \psi(x)\exp\Big(-\frac{i2\pi mx}{L}\Big) = \frac{1}{L}\sum_{n\in\boldsymbol{N}}\Big[\int_{-L/2}^{L/2}\exp\Big(\frac{i2\pi(n-m)x}{L}\Big)\Big]a_n = \delta_{nm}a_n$$

## 10 Lecture 10 (April 7th)

**Recall.** In the most general case, we model states of quantum mechanical system as a complex Hilbert space (a vector space that is complete with respect to its inner product). In this regard, a wave function

**Chapter 4** 1-dimensional Potential Problem

**Remark.** We solve the following boundary value problem with various potential functions:

$$H\psi(x) = E\psi(x) \quad \text{with} \quad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Some examples of potential functions are steps, wells, barriers, delta functions, and simple harmonic oscillators.

**Theorem.** (Step function)

$$V(x) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0 \end{cases}$$

*Proof.* We impose that

(i) (continuous at zero) $\psi(x \to 0^-) = \psi(x \to 0^+)$

(ii) (derivative is continuous at zero) $\psi'(x \to 0^-) = \psi'(x \to 0^+)$

Imposing these two conditions we have a general solution

$$\psi(x) = \begin{cases} e^{ikx} + Re^{-ikx} & x < 0 \\ Te^{iqx} & x > 0 \end{cases}$$

with $k^2 = 2mE/\hbar^2$ and $q^2 = 2m(E - V_0)/\hbar > 0$. With the conditions

$$\begin{cases} 1 + R = T \\ ik(1 - R) = iqT \end{cases}$$

we find

$$\begin{cases} R = \dfrac{k-q}{k+q} \\ T = \dfrac{2k}{k+q} \end{cases}$$

Therefore with all $E > V_0$, solutions exist. We have previously defined the current density:

$$\mathbf{J}(x) = \frac{\hbar}{2im}(\psi^* \nabla \psi - \nabla \psi^* \psi)$$

Using the definition of current density as density times velocity,

$$\frac{\hbar k}{m}(1 - |R|^2) = |T|^2 \frac{\hbar q}{m}$$

we notice that the first condition along with this condition also gives the same solutions for $R$ and $T$. For another situation, we have

$$\begin{cases} 1 + R = T \\ ik(1 - R) = -q'T \end{cases}$$

with solutions

$$\begin{cases} R = \dfrac{ik + q'}{ik - q;} \\ T = \dfrac{2k}{k + iq'} \end{cases}$$

with $|R|^2 = 1$. Notice how $T$ does not vanish. $\square$

## 11 Lecture 11 (April 9th)

Today, we will deal with the potential well.

**Theorem.** Consider the potential well problem.

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

For this,

$$\begin{cases} E < -V_0: & \text{no solutions} \\ -V_0 < E < 0: & \text{bound state} \\ 0 < E: & \text{scattering state} \end{cases}$$

We will deal the last case first, which we call the scattering state. Then,

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

and

$$\begin{cases} |x| > a & \psi'' + k^2\psi = 0 \\ |x| < a & \psi'' + q^2\psi = 0 \end{cases}$$

for $k^2 = 2mE/\hbar^2$ and $q^2 = 2m(E + V_0)/\hbar^2$. Then,

$$\begin{cases} x < -a & e^{ikx} + Re^{-ikx} \\ -a < x < a & Ae^{iqx} + Be^{-iqx} \\ a < x & Te^{ikx} \end{cases}$$

To obtain the coefficients, we can impose either that the wave function and its derivative is continuous or that

(i) (Continuity of logarithm)
$$\frac{1}{\psi}\frac{\partial \psi}{\partial x} = \frac{\partial}{\partial x}(\ln \psi)$$

(ii) $\mathbf{J}(x)$ is continuous

From (ii) we have, at $x = a$,

$$\frac{\hbar k a}{m}(1 - |R|^2) = \frac{\hbar q}{m}(|A|^2 - |B|^2) = \frac{\hbar k}{m}|T|^2$$

The point is that we have four equations, two for $x = a$ and two for $x = -a$. In conclusion, we have

$$\begin{cases} R = \dfrac{ie^{-2ika}(q^2 - k^2)\sin 2qa}{2kq\cos 2qa - i(q^2 + k^2)\sin 2qa} \\ T = \dfrac{e^{-2ika}2kq}{2kq\cos 2qa - i(q^2 + k^2)\sin 2qa} \end{cases}$$

The fact that the $\sin 2qa$ exists on the numerator of $R$ is rather shocking as when $4qa = n(s\pi)$ we have $R = 0$. This can be understood through the wave property of the particle. This was vigourously studied in Ramsauer-Townsend resonance.

**Theorem.** Consider the barrier problem.

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

Then,

$$\psi'' + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad \psi'' - \kappa^2\psi = 0$$

with $\kappa^2 = 2m(V_0 - E)/\hbar$. We have the ansatz

$$\begin{cases} x < -a & e^{ikx} + Re^{-ikx} \\ -a < x < a & Ae^{-\kappa x} + Be^{\kappa x} \\ x > a & Te^{ikx} \end{cases}$$

The story is the same, with two values each at $-a$ and $a$. We have the following simultaneous equations.

(i) ($\psi$ continuity at $x = -a$) $e^{-ika} + Re^{ika} = Ae^{\kappa a} + Be^{-\kappa a}$

(ii) ($\psi$ continuity at $x = a$) $Ae^{-\kappa a} + Be^{\kappa a} = Te^{ika}$

(iii) ($\psi'$ continuity at $x = -a$) $ike^{-ika} + R(-ik)e^{ika} = -\kappa Ae^{\kappa a} + B\kappa e^{-\kappa a}$

(iv) ($\psi'$ continuity at $x = a$) $-\kappa Ae^{-\kappa a} + \kappa Be^{\kappa a} = ikTe^{ika}$

We arrive at

$$\begin{cases} |T|^2 = \dfrac{(2\kappa k)^2}{(2k\kappa)^2\cosh^2(2\kappa a) + (k^2 - \kappa^2)^2\sinh^2(2\kappa a)} \\ |R|^2 = \dfrac{(k^2 + \kappa^2)\sinh^2(2\kappa a)}{(2k\kappa)^2 + (k^2 + \kappa^2)^2\sinh^2(2\kappa a)} \end{cases}$$

where $\cosh^2 x - \sinh^2 x = 1$. Notice flux conservation, $|R|^2 + |T|^2 = m/\hbar k$. We naturally question whether flux conservation satisfies in the barrier itself. Applying the formula for probability flux,

$$j = \frac{\hbar}{2im}\Big(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\Big)$$
$$= \frac{\hbar}{2im}2\kappa(-AB^* + A^*B) = \frac{\hbar k}{m}|T|^2$$

When $x$ is larger than 1, we can aproximate $\sinh x \sim e^x/2$ and we can approximate the transmission constant squared as

$$|T|^2 \sim Ce^{-2(\kappa 2a)}$$

for some constant $C$. $2a$ symbolises the barrier's width and we know that $\kappa = 2m\sqrt{(V_0 - E)}/\hbar^2$. As such, we understand that as the barrier's width increases, the probability that the particle penetrates it exponentially decreases. More generally, for an arbitrary potential function,

$$|T|^2 \sim C\exp\Big(-2\int_{x_1}^{x_2}\frac{2m}{\hbar^2}\sqrt{V(x) - E}\Big)$$

## 12 Lecture 12 (April 14th)

**Remark.** We previously studied the case where the total energy was less than the potential barrier ($E < V_0$). In a general case, we can consider a barrier as a composition of step barriers. The transmission coefficient then follows the following proportionality:

$$|T|^2 \propto \exp\Big(-2\int_{x_1}^{x_2}\sqrt{\frac{2m}{\hbar^2}(V(x) - E)}\Big)$$

where $x_1$ and $x_2$ are the endpoints of the barrier. This should definitely be memorised.

**Example.** Consider a metal apparatus where an electric field of magnitude $\varepsilon$ is applied. The potential energy is given by $V(x) = -x(e\varepsilon)$. A electron at zero energy, the potential energy is then given by $W - x(e\varepsilon)$ where $W$ is thework-function of the metal. Then, from the above equation,

$$|T|^2 \propto \exp\Big(-2\int_0^a\sqrt{\frac{2m}{\hbar^2}(W - x(e\varepsilon))}\Big) = \exp\Big(-\frac{4\sqrt{2}}{3}\sqrt{\frac{mWa^2}{\hbar^2}}\Big)$$

with $W/e\varepsilon = a$. This equation is called the Fowler-Nordheim equation. For the potential well, the scattering state can be considered as unbounded orbital motion while the bounded state can be considered as bounded orbital motion. When it comes to bounded states, parity symmetry is important, as the potential function is a symmetric function $V(x) = V(-x)$. This implies that the eigenfunctions $\psi(x)$ are also even or odd. It now suffices to consider the boundary condition only at $x = a$.

$$\psi'' + \frac{2m}{\hbar}(E - V(x))\psi = 0$$

Then,

$$\begin{cases} a < x \quad \alpha^2 = \dfrac{2m}{\hbar}(-E) 0 \leq x < a \quad \dfrac{2m}{\hbar}(E + V_0) \end{cases}$$

we then have $\psi \propto e^{-\alpha x}$ and $\psi \propto (\sin qx, \cos qx)$ as general ansatz. Requiring the continuity of $\psi'/\psi$ at $a$ for the even (odd) part,

$$-\frac{\alpha e^{-\alpha x}}{e^{-\alpha x}}\Big|_{a^+} = \frac{-q \sin qx}{\cos qx}\Big|_{a^-}$$

and we have $\alpha a = q \tan qa$ for even and $\alpha a = -q \cot qa$ for the odd part of the function. Notice how $y = qa$ and $\lambda = 2mV_0 a^2/\hbar^2$ are dimensional quantities that we shall now define. We can then obtain for the even case

$$\frac{\sqrt{\lambda - y^2}}{y} = \tan y$$

and for the odd case

$$\frac{\sqrt{\lambda - y^2}}{y} = -\cot y$$

From this we get that for large $\lambda$, we get more solutions. Note that in the ground state, the solution must have an even parity.

**Theorem.** Another interesting apparatus is the double well. As asymmetric potential functions are a result of a composition of even and odd functions with different energy values, it cannot be

## 13 Lecture 13 (April 16th)

**Theorem.** Last class we've learned that in the double well problem, the ground state is given by an even solution. The odd solution would then be an excited state. The superposition of the two ($\psi_e - \psi_o$ or $\psi_e + \psi_o$) gives a asymmetrical distribution. Let's say that the wave function is initially in the right:

$$\begin{aligned} \psi(t > 0) &= \exp\Big(-\frac{iE_e t}{\hbar}\Big)\psi_e(x) + \exp\Big(-\frac{iE_0 t}{\hbar}\Big)\psi_o(x) \\ &= \exp\Big(-\frac{iE_e t}{\hbar}\Big)\Big(\psi_e + \exp\Big[-\frac{i(E_o - E_e)t}{\hbar}\Big]\psi_o\Big) \end{aligned}$$

Given that $E_o > E_e$, we notice that when

$$\frac{E_o - E_e}{\hbar} t' = \pi$$

the sign of the function flips and the wave function moves to the left.

**Theorem.** (Potential problem for dirac distribution) Consider the potential

$$V(x) = -\frac{\hbar^2}{2m}\frac{\lambda}{a}\delta(x)$$

where $\lambda$ is a dimensionless constant. The Schrodinger equation is

$$\psi'' - \kappa^2\psi = -\frac{\lambda}{a}\delta(x)\psi$$

where $-\kappa^2 = 2mE/\hbar$.

$$\begin{cases} x > 0 & c_1 e^{-\kappa x} \\ x < 0 & c_2 e^{\kappa x} \end{cases}$$

We require that the wave function is continuous at $x = 0$, and discover that $c_1 = c_2 = c$. What about the derivative at $x = 0$? The technique is to integrate the differential equation in a small ball around the origin.

$$\int_{-\varepsilon}^{\varepsilon} dx\ \psi'' - \int_{-\varepsilon}^{\varepsilon} dx\ \kappa^2\psi = -\frac{\lambda}{a}\int_{-\varepsilon}^{\varepsilon} dx\ \delta(x)\psi(x)$$

We then have

$$\begin{aligned} \psi'(x = 0^+) - \psi'(x = 0^-) =& \frac{\lambda}{a}\psi(0) \\ c(-\kappa) - c(\kappa) =& -c\frac{\lambda}{a} \end{aligned}$$

which allows us to have a single solution with $2\kappa = \lambda/a$. Two good exercises is when there is a double delta function well and there is a positive delta function barrier (this is in the test)!

**Definition.** (Harmonic oscillator) (important) The Hamiltonian of a harmonic oscillator is given as

$$\hat{H}\psi(x) = \Big(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\Big)\psi(x) = E\psi(x)$$

Note that $\varepsilon = 2E/\hbar\omega$ and $y = \sqrt{mx/\hbar x}$ are dimensionless constants (check this). Then,

$$\frac{d^2\psi}{dy^2} + (\varepsilon - y^2)\psi = 0$$

is an adjoint operator as $c_0' = c_1 = 0$. When $y$ is large, the $\varepsilon$ term can be ignored.

Multiplying $\psi_0'$ to both sides,

$$\begin{aligned}\psi_0'\psi_0'' - y^2\psi_0\psi_0' =&0\\ \frac{d}{dy}[(\psi_0')^2 - y^2\psi_0^2] =& -2y\psi_0^2\end{aligned}$$

at this point, we can impose that $\psi \to 0$ and fastly and $|y| \to \infty$ and say:

$$(\psi_0')^2 - y^2\psi_0^2 = c$$

implying that

$$\frac{d\psi_0}{dy} = \pm\sqrt{c + y^2\psi_0^2} = -y\psi_0$$

As imposing boundary conditions, we find $c = 0$ and as we want an exponential decay, we choose the negative sign. We find

$$\psi_0 = e^{-y^2/2}$$

Setting $\psi(y) = e^{-y^2/2}h(y)$ as our ansatz we find

$$h'' - 2yh' + (\varepsilon - 1)h = 0$$

Notice that this is a Hermite differential equation. We can choose the following idicial equation near $y = 0$

$$h(y) = \sum_{j=0}^{\infty} y^k y^j a_j$$

We then obtain

$$0 = \sum_{j=0}^{\infty}(k+j)(k+j-1)a_j y^{k+j-2} + \sum_{j=0}^{\infty}\Big[-2(k+j) + (\varepsilon - 1)\Big]a_j y^{k+1}$$

where $j = 0, 1$ have no matching indexes. We then consider these separately, arriving at an indicial equation ($a_0 \neq 0$ is obvious). For $k = 0, 1$ we have

$$\begin{cases} j = 0 & 0 = k(k-1)a_0 \\ j = 1 & 0 = (k+1)ka_1 \end{cases}$$

$$0 = \sum_{j=0}^{\infty}(k+j)(k+j-1)a_{j+2} y^{k+j} + \sum_{j=0}^{\infty}\Big[-2(k+j) + (\varepsilon - 1)\Big]a_j y^{k+j}$$

We arrive at a recurrence equation,

$$a_{j+2} = \frac{2(k+j) - (\varepsilon - 1)}{(k+j+2)(k+j+1)}a_j$$

When $k = 0$,

$$
\begin{aligned}
a_2 =& \frac{2(0 - (\varepsilon - 1)/2)}{2 \cdot 1} a_0 \\
a_4 =& \frac{2^2}{4!}\Big(2 - \frac{(\varepsilon - 1)}{2}\Big)\Big(0 - \frac{(\varepsilon - 1)}{2}\Big) a_0
\end{aligned}
$$

When $k = 1$,

$$
\begin{aligned}
a_2 =& 2 - \frac{1 - (\varepsilon - 1)/2}{2 \cdot 3} a_0 \\
a_4 =& \frac{2^2}{5!}\Big(3 - \frac{(\varepsilon - 1)}{2}\Big)\Big(1 - \frac{(\varepsilon - 1)}{2}\Big)
\end{aligned}
$$

For an arbitrary $\varepsilon$, such a sequence explodes, and we must choose a special $\varepsilon$ and truncate the infinite series. In the case that $k = 0$, we truncate when

$$
\frac{\varepsilon - 1}{2} = 0, 2, 4, \ldots
$$

and in the case that $k = 1$, we truncate when

$$
\frac{\varepsilon - 1}{2} = 1, 3, 5, \ldots
$$

## 14 Lecture 15 (April 30th)

**Chapter 5** Essential Elements

**Definition.** (Quantum State) A pure quantum state is defined as a ray in a Hilbert space. Here, a Hilbert space is a complex vector space with the inner product that is a complete. Some examples of Hilbert spaces are $L^2$, $\boldsymbol{C}^n$, and $M_{n\times n}$

**Definition.** (Ray) By a ray, we mean that for $|\psi\rangle \in \mathcal{H}$, $\{c|\psi\rangle\}$ where $c \in \mathcal{C}$. As we are considering normalised wave functions, $\langle\psi|\psi\rangle = 1$ and $|c|^2\langle\psi|\psi\rangle = 1$ and $|c|^2 = 1$, leading to $c = e^{i\theta}$ and $\{e^{i\theta}\psi\}$. This is saying that a state is equivalent up to a transformation that conserves the modulus.

**Definition.** (Composite system) Consider two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. In the discussion of a system comprised of both Hilbert spaces, we necessarily look at bilinear maps. A composite system of quantum states is therefore expressed as a tensor product

$$
|\psi\rangle_1 \otimes |\psi\rangle_2 \in \mathcal{H}_1 \otimes \mathcal{H}_2
$$

When an element in such a tensor product can be expressed as a tensor product like the above, we say that such an element is separable. If not, we say that the element is entangled.

**Example.** (Kronecker product) We can consider the Kronecker product as a specific example of a tensor product. Let

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad B = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

We can use the representation

$$A \otimes B = \begin{pmatrix} aB & bB \\ cB & dB \end{pmatrix} = \begin{pmatrix} a\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} & b\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \\ \\ c\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} & d\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \end{pmatrix}$$

**Example.** Now, let $A = (x, y)$ and $B = (a, b)$. Then,

$$A \otimes B = (xB, yB) = \begin{pmatrix} xa & ya \\ xb & yb \end{pmatrix}$$

Also,

$$B \otimes A = \begin{pmatrix} a(x, y) \\ b(x, y) \end{pmatrix} = \begin{pmatrix} ax & ay \\ bx & by \end{pmatrix}$$

**Definition.** (Observables, their adjoint, and their expectation) An operator is a linear function from a Hilbert space to the complex numbers (linear map).

$$\hat{O} : \mathcal{H} \to \boldsymbol{C}$$

An adjoint of an operator is an operator that satisfies (we often denote $\hat{O}|\psi\rangle = |\hat{O}\psi\rangle$)

$$\langle \hat{O}\phi|\psi\rangle = \langle \phi|\hat{O}^\dagger|\psi\rangle$$

where $\hat{O}^\dagger$ is the adjoint. Notice how

$$\langle \hat{O}\phi|\psi\rangle^* = \langle \psi|\hat{O}\phi\rangle = \langle \hat{O}^\dagger\psi|\phi\rangle = \langle \phi|\hat{O}^\dagger\psi\rangle^*$$

and that the definition for an adjoint operator can also be written as

$$\langle \hat{O}^\dagger\phi|\psi\rangle = \langle \phi|\hat{O}|\psi\rangle$$

Now, for the expectation value for a measurement to be real, we have

$$\langle \psi|\hat{O}|\psi\rangle = \langle \psi|\hat{O}|\psi\rangle^* = \langle \hat{O}\psi|\psi\rangle = \langle \psi|\hat{O}^\dagger|\psi\rangle$$

That is, for an expectation value for a measurement to be real, the observable must be

Hermitian.

## 15 Lecture 16 (March 5th)

(Online lecture on partial differential equations)

## 16 Lecture 17 (May 7th)

**Definition.** (Adjointness as a suffient condition for real eigenvalues) An adjoint operator is defined as

$$\langle\psi|A^\dagger|\phi\rangle = \langle A\psi|\phi\rangle$$

Where a self-adjoint operator is an operator that satisfies

$$A = A^\dagger$$

We have previously seen how the following inner product is real if self-adjointness holds.

$$\langle\psi|A|\psi\rangle$$

**Theorem.** (Completeness relation) A basis is complete if and only if the completeness relation holds.

$$\mathbf{1} = \sum_n |n\rangle\langle n|$$

*Proof.* Suppose that a Hilbert space has a complete orthonormal basis satisfying $\langle n|m\rangle = \delta_{nm}$. For $|\psi\rangle \in \mathcal{H}$, we have the following representation.

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

The coefficients are given by

$$\langle m|\psi\rangle = \sum_n c_n\langle m|n\rangle = c_m \quad \text{and} \quad |\psi\rangle = \sum_n \langle n|\psi\rangle|n\rangle = \sum_n |n\rangle\langle n|\psi\rangle$$

From the above, we have

$$\mathbf{1} = \sum_n |n\rangle\langle n|$$

which is called the completeness relation. Conversely, we can assume that the above is true for any $|\psi\rangle$, and any vector could be expanded in terms of the basis. We have thus proved the theorem. □

**Definition.** (Dual spaces and the Riesz Lemma) The dual space of a vector space $V$ is the vector space that contains all the linear maps $T : V \to \boldsymbol{C}$ that act on $V$. There is a one-to-one correspondence between the dual space and the inner products $\langle \cdot | w \rangle$ and moreover the dual space and $V$.

$$\underbrace{\langle\psi|}_{\text{bra}} \longleftrightarrow \underbrace{|\psi\rangle}_{\text{ket}} \quad \text{and} \quad \langle\psi|A^\dagger \longleftrightarrow A|\psi\rangle$$

Notice that from $\langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle$, we can deduce the conjugate linearity of the first argument. Consider how

$$\langle\beta|c_1v_1 + c_2v_2\rangle = c_1\langle\beta|v_1\rangle + c_2\langle\beta|v_2\rangle$$
$$\langle c_1v_1 + c_2v_2|\beta\rangle = c_1^*\langle v_1|\beta\rangle + c_2^*\langle v_2|\beta\rangle$$

**Definition.** (Operator algebra) Notice that operators form a ring with an underlying structure of a vector space which is exactly the definition of an algebra.

**Remark.** (Identities)

(i) $(A^\dagger)^\dagger = A$

(ii) $(AB)^\dagger = B^\dagger A^\dagger$

(iii) $(\alpha A)^\dagger = \alpha^* A^\dagger$

*Proof.* For (i), let $B = A^\dagger$.

$$\langle\phi, B^\dagger\psi\rangle = \langle B\phi, \psi\rangle = \langle\psi, B\phi\rangle^* = \langle\psi, A^\dagger\phi\rangle^* = \langle A\psi, \phi\rangle^* = \langle\phi, A\psi\rangle$$

This will be on the test! For (ii),

$$\langle\phi, (AB)^\dagger\psi\rangle = \langle AB\phi, \psi\rangle = \langle B\phi, A^\dagger\psi\rangle = \langle\phi, B^\dagger A^\dagger\psi\rangle$$

For (iii),

$$\langle\phi, (\alpha A)^\dagger\psi\rangle = \langle\alpha A\phi, \psi\rangle = \alpha^*\langle A\phi, \psi\rangle = \alpha^*\langle\phi, A^\dagger\psi\rangle$$

□

**Theorem.** (Eigenvalue problem for Hermitian operators) Let $A|\psi_n\rangle = a_n|\psi_n\rangle$ and $A|\psi_m\rangle = a_m|\psi_m\rangle$. Applying the dual of $|\psi_m\rangle$ and $|\psi_n\rangle$ each,

$$\langle\psi_m|A|\psi_n\rangle = a_n\langle\psi_m|\psi_n\rangle \quad \langle\psi_n|A|\psi_m\rangle = a_m\langle\psi_n|\psi_m\rangle$$

Taking the complex conjugate of the right, we have

$$\langle\psi_m|A^\dagger|\psi_n\rangle = \langle A\psi_m|\psi_n\rangle = \langle\psi_n|A\psi_m\rangle^* = a_m^*\langle\psi_m|\psi_n\rangle$$

We conclude that

$$a_m^* \langle \psi_m | \psi_n \rangle = a_n \langle \psi_m | \psi_n \rangle \quad \text{and} \quad (a_m^* - a_n) \langle \psi_m | \psi_n \rangle = 0$$

when $m = n$, due to the positive definiteness of the inner product, we conclude that the eigenvalues are real. When $m \neq n$, we require that the inner product is zero, which proves orthogonality. In conclusion, we have proved the for self-adjoint operators, eigenvalues are real and they form an orthonormal set. Whether they form a complete basis is another difficult problem which we take for granted.

**Proposition.** (Probability interpretation) For an observable quantity $A$ measured with respect to $|\psi\rangle$, once a observation is made, one of $\{a_n\}$ is observed and the probability that this happens is $|a_n|^2$.

## 17 Lecture 18 (May 12th)

**Proposition.** The dynamics, or evolution of a quantum state is given by

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

whereas, because $\hat{H} = \hat{H}^\dagger$,

$$-i\hbar \frac{\partial}{\partial t} \langle \psi(t)| = \langle \psi(t)| \hat{H}$$

**Definition.** For any linear map $\hat{A} : V \to V$ between vector spaces, we can create a matrix representation according to

$$\hat{A}(\mathbf{e}_i) = \sum_j \mathbf{e}_j A_{ji} \quad \text{and} \quad \langle \mathbf{e}_j, \hat{A}(\mathbf{e}_i) \rangle = \sum_k A_{ki} \langle \mathbf{e}_j, \mathbf{e}_k \rangle = \sum_k A_{ki} \delta_{jk} = A_{ji}$$

with respect to the basis $\{\mathbf{e}_i\}$. Now, let $\mathcal{H}$ be a Hilbert space with respect to $\{|n\rangle\}$. For an operator $\hat{A} : \mathcal{H} \to \mathcal{H}$, we have

$$\hat{A}|n\rangle = \sum_n A_{mn} |m\rangle \quad \text{or} \quad \langle m | \hat{A} | n \rangle = A_{mn}$$

Now, by extension, we can create a matrix representation for any operator by employing the completeness relation

$$\hat{A} = \mathbf{1} \hat{A} \mathbf{1} = \sum_{n,m} |n\rangle \langle n | \hat{A} | m \rangle \langle m| = \sum_{m,n} A_{nm} |n\rangle \langle m|$$

In the language of matrices, for any inner product, we can express

$$\langle\Phi|\Psi\rangle = \langle\Phi|\sum_n |n\rangle\langle n|\Psi\rangle = \sum_n \langle\Phi|n\rangle\langle n|\Psi\rangle = \sum_n (\langle 1|\Phi\rangle^*, \langle 2|\Phi\rangle^*, \ldots) \begin{pmatrix} \langle 1|\Psi\rangle \\ \langle 2|\Psi\rangle \\ \vdots \end{pmatrix}$$

Therefore, kets can be seen as column vectors while bras can be seen as complex conjugated and transposed rows. Likewise, the dual relationship between the Hermitian and row vectors are parallel to the dual relation between bras and kets.

**Example.** (Quantum gates) We now learn the NOT quantum gate $\hat{O} : \mathbf{C}^2 \to \mathbf{C}^2$. If suffices to define the linear function on the basis like the following:

$$\begin{cases} \hat{O}|0\rangle = |1\rangle \\ \hat{O}|1\rangle = |0\rangle \end{cases}$$

We can now find the matrix representation using the formalism above,

$$\begin{aligned} A_{11} = \langle 0|\hat{O}|0\rangle = 0 \quad A_{12} = \langle 0|\hat{O}|1\rangle = 1 \\ A_{21} = \langle 1|\hat{O}|0\rangle = 1 \quad A_{22} = \langle 1|\hat{O}|1\rangle = 0 \end{aligned}$$

Where we get

$$\hat{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{or} \quad \hat{A} = |1\rangle\langle 0| + |0\rangle\langle 1|$$

**Definition.** The Pauli matrices are defined like the following

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that they are Hermitian, unitary, and has a trace of 0.

**Definition.** (Mixed state) A general (or mixed) quantum state $\rho : \mathcal{H} \to \mathcal{H}$ is defined as an operator that is

(i) Hermitian

(ii) $\mathrm{Tr}(\rho) = 1$

(iii) Positive operator (also called a positive semidefinite operator), meaning $\langle\psi|\rho|\psi\rangle \geq 0$ for all $|\psi\rangle$

A general quantum state is also called a density operator.

**Definition.** In the Dirac sense, the wavefunctions $\psi(x)$ and $\phi(x)$ in the position space and the momentum space respectively are the coefficents of the state vector when projected into the position space and momentum space respectively. That is, by defining the eigenstates

$|x\rangle$ and $|p\rangle$ to form a generalised orthonormal basis satisfying the following condition,

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

states can be expanded as

$$|\psi\rangle = \int_{-\infty}^{\infty} dx'\, \psi(x')|x'\rangle \quad |\psi\rangle = \int_{-\infty}^{\infty} dp'\, \phi(p')|p'\rangle$$

with

$$\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx'\, \psi(x')\langle x|x'\rangle = \int_{-\infty}^{\infty} dx'\, \psi(x')\delta(x - x') = \psi(x)$$

and likewise for the momentum function.

## 18 Lecture 19 (May 14th)

**Lemma.** We first try to obtain $\langle x|p\rangle$ and $\langle p|x\rangle$. Notice that

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle = -i\hbar \frac{d}{dx}\langle x|p\rangle$$

Solving the differential equation we find

$$\langle x|p\rangle = A(p)e^{ipx/\hbar}$$

Noting the identity

$$\int_{-\infty}^{\infty} dx\, e^{ikx} = 2\pi\delta(k)$$

we find

$$\begin{aligned}
\langle p|p'\rangle &= \delta(p - p') \\
\int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|p'\rangle &= \delta(p - p') \\
\int_{-\infty}^{\infty} dx\, |A(p)|^2 e^{ix(p-p')/\hbar} &= \delta(p - p') \\
|A(p)|^2 2\pi\delta\Big(\frac{p - p'}{\hbar}\Big) &= \delta(p - p') \\
A(p) = \frac{1}{\sqrt{2\pi\hbar}}
\end{aligned}$$

**Theorem.** (Fourier transform) We find that the inverse Fourier and Fourier transforms are given as

$$\psi(x) = \langle x|\psi\rangle = \int_{-\infty}^{\infty} dp\, \langle x|p\rangle\langle p|x\rangle$$
$$= \int_{-\infty}^{\infty} dp\, e^{ipx/\hbar}\frac{1}{\sqrt{2\pi\hbar}}\phi(p)$$

and

$$\phi(p) = \langle p|\psi\rangle = \int_{-\infty}^{\infty} dx\, e^{ipx/\hbar}\frac{1}{\sqrt{2\pi\hbar}}\psi(x)$$

**Remark.**
**Proposition.** (Matrix representation) We can express the below basis independent expression of an arbitrary linear transformation in terms of matrices,

$$|\psi\rangle = A|\phi\rangle$$

by projecting into the basis $\langle m|$ and inserting the completeness relation,

$$\langle m|\psi\rangle = \sum_n \langle m|A|n\rangle\langle n|\phi\rangle \quad \text{or} \quad \psi_m = \sum_n A_{mn}\phi_n$$

where $\phi_m$ and $\phi_n$ are ordinary matrices. On the other hand,

$$A = BC$$

can be expressed as

$$\langle m|A|n\rangle = \sum_k \langle m|B|k\rangle\langle k|C|n\rangle \quad \text{or} \quad A_{mn} = \sum_k B_{mk}C_{kn}$$

**Remark.** (Adjoint matrices) We now seek the matrix expression for an adjoint operator.

$$(A_{nm})^\dagger = \langle n|A^\dagger|m\rangle = \langle An|m\rangle = \langle m|An\rangle^* = (\langle m|A|n\rangle)^* = A^*_{mn}$$

We find that an adjoint of an operator in terms of its matrix is simply the complex transpose of the operator itself.

**Definition.** (Unitary operators) A key property of unitary operators (operators satisfying $O^\dagger O = OO^\dagger = \mathbf{1}$) is that they preserve inner products. This can be seen from the fact that as $|\phi\rangle \to U|\phi\rangle$ and $|\psi\rangle \to U|\psi\rangle$,

$$\langle U\psi|U\phi\rangle = \langle\psi|U^\dagger U|\phi\rangle$$

**Definition.** (Trace) The trace of a matrix is defined like the following

$$\mathrm{Tr}(A) = \sum_n \langle n|A|n\rangle = \sum_n A_{nn}$$

However, see how the definition relies of a certain basis $\{|n\rangle\}$. We now prove that the definition is independent on this set. Take another basis $\{|m\rangle\}$. We see that

$$\begin{aligned}\sum_n \langle n|A|n\rangle &= \sum_{n,m_1,m_2} \langle n|m_1\rangle\langle m_1|A|m_2\rangle\langle m_2|n\rangle \\ &= \sum_{n,m_1,m_2} \langle m_1|A|m_2\rangle\langle m_2|n\rangle\langle n|m_1\rangle \\ &= \sum_{m_1,m_2} \langle m_1|A|m_2\rangle\delta_{m_1m_2}\end{aligned}$$

**Definition.** (Spectral decomposition of a Hermitian operator) Consider a Hermitian operator

$$\hat{A} = \sum_{n,m} |n\rangle\langle n|A|m\rangle\langle m|$$

and select the basis to be eigenkets of $\hat{A}$. We have

$$\langle n|\hat{A}|m\rangle = \langle n|A_m|m\rangle = A_m\langle n|m\rangle = A_m\delta_{nm}$$

When inserting this into the above, we diagonalise the matrix by obtaining

$$\sum_m |m\rangle A_m\langle m|$$

We see that the eigenvalues form the diagonals of the Hermitian matrix.

**Theorem.** (Operator solution of the simple harmonic oscillator) We have previously witnessed the simple harmonic oscillator whose Hamiltonian was given by

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

We are certain that $\langle\psi|\hat{H}|\psi\rangle \geq 0$ from the fact that $\langle\psi|\hat{x}\hat{x}|\psi\rangle = \langle\hat{x}^\dagger\psi|\hat{x}\psi\rangle \geq 0$. Define the following operator

$$\begin{aligned}\hat{a} &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\omega\hbar}} \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}\end{aligned}$$

If possible, memorise these. Knowing that $[\hat{x}, \hat{p}] = i\hbar$, we can compute that $[\hat{a}, \hat{a}^\dagger] = \mathbf{1}$. We then find

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \quad \hat{p} = \dots$$

In terms of $\hat{a}$, we therefore find the Hamiltonian above to be (it is extremely important to be careful of the order of $\hat{a}$ and $\hat{a}^\dagger$):

$$\hbar\omega\Big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\Big)$$

What is the commutator relation between $\hat{H}$ and $\hat{a}$? We see that

$$[H, a] = \hbar\omega\Big[a^\dagger a + \frac{1}{2}a\Big] = \hbar\omega(a^\dagger[a, a] + [a^\dagger, a]a) = \hbar\omega(-a) \quad \text{with} \quad [H, a^\dagger] = \hbar\omega a^\dagger$$

Physically, each operator is defined as operators that raise and lowers energy levels. Now we actually solve for energy levels.

$$\hat{H}|E\rangle = E|E\rangle$$
$$\hat{H}(a|E\rangle) = (aH + [\hat{H}, a])|E\rangle = (\hat{a}E - \hbar\omega\hat{a})|E\rangle = (E - \hbar\omega)(\hat{a}|E\rangle)$$

## 19 Lecture 20 (May 19th)

**Theorem.** Let there be an energy state $\hat{H}|E\rangle = E|E\rangle$. We previously found how

$$\hat{H}(\hat{a}|E\rangle) = (E - \hbar\omega)(\hat{a}|E\rangle)$$

and

$$\hat{H}(a^\dagger|E\rangle) = (E + \hbar\omega)(\hat{a}^\dagger|E\rangle)$$

Which needs to be verified. We have previously proved

$$\langle\psi|\hat{H}|\psi\rangle \geq 0$$

and tells us that there is a limit to how much the energy can be lowered. We thus define

$$\hat{a}|0\rangle = \mathbf{0}$$

as the ground state, where $\mathbf{0}$ is the zero vector. A simple corollary would be that

$$\hat{H}|0\rangle = (\hbar\omega)(\hat{a}^\dagger\hat{a})|0\rangle = \frac{1}{2}\hbar\omega|0\rangle$$

telling us that the ground state has an energy of $\hbar\omega/2$. We can apply the creation operator to obtain higher energy states:

$$H(\hat{a}^\dagger|0\rangle) = \Big(\frac{1}{2}\hbar\omega + \hbar\omega\Big)(\hat{a}^\dagger|0\rangle)$$

For arbitrary states,

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

and

$$|n\rangle = c_n (\hat{a}^\dagger)^n |0\rangle$$

We now prove that these eigenvectors form an orthonormal basis. The inner product of two eigenstates are

$$\langle m|n\rangle = c_m^* c_n \langle 0|a^m (a^\dagger)^n|0\rangle = c_m^* c_n n\langle 0|a^{m-1}(a^\dagger)^{n-1}|0\rangle$$

as $a^{m-1}a(a^\dagger)^n = ((a^\dagger)^n)a + [a,(a^\dagger)^n]) = ((a^\dagger)^n a + n(a^\dagger)^{n-1})$. Therefore, when $n \neq m$, we find $\langle n|m\rangle = 0$ and if they are equal,

$$\langle n|m\rangle = |c_n|^2 n\langle 0|a^{n-1}(a^\dagger)^{n-1}|0\rangle = |c_n|^2 n(n-1)\langle 0|a^{n-1}(a^\dagger)^{n-2}|0\rangle = \ldots = |c_n|^2 n!\langle 0|0\rangle = 1$$

thus getting something we should definitely memorise,

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

with $\langle n|m\rangle = \delta_{nm}$. Let's not find the annihilator operators matrix representation.

$$\begin{aligned}\langle m|a|n\rangle =& \langle m|a\cdot\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle = \frac{1}{\sqrt{n!}}\langle m|(a^\dagger)^n a + a(a^\dagger)^n|0\rangle\\ =& \frac{n}{\sqrt{n!}}\langle m|(a^\dagger)^{n-1}|0\rangle = \frac{n}{\sqrt{n!}}\sqrt{(n-1)!}\langle m|\frac{(a^\dagger)^{n-1}}{\sqrt{(n-1)!}}|0\rangle\\ =& \sqrt{n}\,\delta_{m,n-1}\end{aligned}$$

We can use the above to also obtain the creator operator's matrix representation, where

$$\langle m|\hat{a}^\dagger|n\rangle = \langle \hat{a}m|n\rangle = \langle n|a|m\rangle^* = (\delta_{n,m-1}\sqrt{m})^* = \delta_{n,m-1}\sqrt{m} = \delta_{m+1,n}\sqrt{n+1}$$

**Theorem.** What is the wavefunction of the ground state? Mathematically, what is $\psi_0 = \langle x|0\rangle$?

$$\hat{a}|0\rangle = 0 \rightarrow \Big(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p}\Big)|0\rangle = 0$$

which leads to

$$\Big[\sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2m\omega\hbar}}\Big(-i\hbar\frac{d}{dx}\Big)\Big]\langle x|0\rangle = 0$$

and

$$\langle x|0\rangle = c\exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)$$

which must be normalised with

$$\int_{-\infty}^{\infty} |\langle x|0\rangle|^2 = 1 \quad \text{and} \quad c = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

To find higher wave functions,

$$\psi_n(x) = \langle x|n\rangle$$

try and compute this with $n = 1$.

**Definition.** Define the exponential of an operator as

$$\exp(\hat{A}) = \sum_{n=0}^{\infty} \frac{1}{n!}(\hat{A})^n$$

Define the operator $\hat{U} = \exp(i\hat{A})$ for a Hermitian $\hat{A}$. We find that

$$\hat{U}^\dagger = (\sum_{n=0}^{\infty}(-i)^n \hat{A}^n) = \exp(-i\hat{A}) = \hat{U}^{-1}$$

Therefore,

$$\hat{U}^\dagger \hat{U} = \mathbf{1}$$

and $\hat{U}$ is a unitary operator.

**Theorem.** (Commuting set of operators and degeneracy) Here, we consider Hilbert spaces that are completely spanned by eigenstates of Hermitian operators. Take

$$\hat{A}|u_a\rangle = a|u_a\rangle$$

which also satisfies

$$\hat{B}|u_a\rangle = b|u_a\rangle$$

Completeness dictates that

$$\sum_{a,b} |u_{ab}\rangle\langle u_{ab}| = \mathbf{1}$$

then,

$$[\hat{A}, \hat{B}]|u_{ab}\rangle = (\hat{A}\hat{B} - \hat{B}\hat{A})|u_{ab}\rangle = (ab - ba)|u_{ab}\rangle = 0$$

telling us that $[\hat{A}, \hat{B}] = 0$.

## 20 Lecture 21 (May 21st)

**Theorem.** (Exsistence of simultaneous eigenkets for commuting operators) Let $[\hat{A}, \hat{B}] = 0$, that is, $\hat{A}$ and $\hat{B}$ be commuting operators. Consider the set of eigenstates $\{|u_a\rangle\}$ of $\hat{A}$, satisfying

$$\hat{A}|u_a\rangle = a|u_a\rangle$$

Observe that

$$\hat{A}(\hat{B}|u_a\rangle) = \hat{B}(\hat{A}|u_a\rangle) = a(\hat{B}|u_a)$$

How many eigenkets (eigenstates) does the eigenvalue $a$ have? Assume that it has 1 and we have:

$$\hat{B}|u_a\rangle = b|u_a\rangle$$

where $|u_a\rangle$ is a simultaneous eigenket for both $\hat{A}$ and $\hat{B}$. In this case, we say that the eigenvalue is nondegenerate. Assume that it has 2, $|u_a^{(1)}\rangle$ and $|u_a^{(2)}\rangle$. Applying the operator $\hat{B}$, we expect

$$\begin{cases} \hat{B}|u_a^{(1)}\rangle = c_{11}|u_a^{(1)}\rangle + c_{21}|u_a^{(2)}\rangle \\ \hat{B}|u_a^{(2)}\rangle = c_{21}|u_a^{(1)}\rangle + c_{22}|u_a^{(2)}\rangle \end{cases}$$

As $\hat{B}$ is Hermitian, the following matrix would have a diagonal form,

$$\begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} \longrightarrow \begin{pmatrix} \lambda_b^{(1)} & 0 \\ 0 & \lambda_b^{(2)} \end{pmatrix}$$

By which we conclude

$$\begin{cases} \hat{B}|v_a^{(1)}\rangle = \lambda_b^{(1)}|v_a^{(1)}\rangle \\ \hat{B}|v_a^{(2)}\rangle = \lambda_b^{(2)}|v_a^{(1)}\rangle \end{cases}$$

for some vectors $|v_a^{(i)}\rangle$. We therefore find $|u_a\rangle$ to be simultaneous eigenkets of $\hat{A}$ and $\hat{B}$. In this case, we say that the eigenvalue is degenerate.

**Definition.** (Expectation values) Consider the expectation value of $\hat{A}$, defined as

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle$$

For kets, the Schrodinger equation is given as

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$
$$-i\hbar\frac{\partial}{\partial t}\langle\psi(t) = \langle\psi(t)|\hat{H}$$

For now, we take $\hat{H}$ to be time-independent. We find

$$\begin{aligned} \frac{d}{dt}\Big(\langle\psi(t)|\hat{A}|\psi(t)\rangle\Big) =& \Big(\frac{d}{dt}\langle\psi(t)|\Big)\hat{A}|\psi(t)\rangle + \langle\psi(t)|A\Big(\frac{d}{dt}|\psi(t)\rangle\Big) + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle \\ =& \frac{i}{\hbar}\langle\psi(t)|[\hat{H},\hat{A}]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle \end{aligned}$$

From this we learn that expectation values (given that the observable is time independent) are only conserved through time when the commutator with the Hamiltonian operator is 0.

$$[\hat{A},\hat{H}] = 0$$

**Example.** (Ehrenfest theorem) Take $\hat{A} = \hat{x}$ and

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

The derivative of the expectation value is given as

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{i}{\hbar}\langle\psi|[H,\hat{x}]|\psi\rangle = \Big\langle\frac{\hat{p}}{m}\Big\rangle$$

On the other hand,

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\langle\psi|[\hat{H},\hat{p}]|\psi\rangle = -\Big\langle\frac{dV}{dx}\Big\rangle$$

Derivating the top equation one more time,

$$m\frac{d^2}{dt^2}\langle\hat{x}\rangle = \frac{d}{dt}\langle\hat{p}\rangle = -\Big\langle\frac{dV}{dx}\Big\rangle$$

we find the quantum mechanical version of Newton's theorem.

**Definition.** (Schrodinger and Heisenberg picture of quantum theory) Like the above, when we take wavefunctions to be time independent, we call the construction Schrodinger's picture of quantum mechanics. On the other hand, suppose that time evolution is introduced by

$$|\psi(t)\rangle = \exp\Big(-\frac{\hat{H}t}{\hbar}\Big)|\psi(0)\rangle$$

where we call the exponential term (an unitary operator) the time evolution operator. The time dependent ket satisfies the Schrodginer equation, as

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = i\hbar\Big(-\frac{i\hat{H}}{\hbar}\Big)\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)|\psi(0)\rangle = \hat{H}|\psi(t)\rangle$$

The expectation value, with this formulation, becomes

$$\langle\psi(0)|\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{A}\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)|\psi(0)\rangle$$

In this case, we see how instead of the states, the operators evolve throughout time ($\hat{A} = \hat{A}(t)$), and quantum mechanics seen in this manner is called Heisenberg's picture. We emphasize that the above is a formal solution, meaning that we aren't caring about details.

In this process, we care about the time derivative of $\hat{A_H}(t)$ which we find to be

$$\begin{aligned}\frac{d}{dt}\hat{A_H}(t) =&\frac{i\hat{H}}{\hbar}\exp\Big(\frac{iHt}{\hbar}\Big)\hat{A}_S\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)+\exp\Big(\frac{iHt}{\hbar}\Big)\hat{A}_S\exp\Big(-\frac{iHt}{\hbar}\Big)\Big(-\frac{i\hat{H}}{\hbar}\Big)\\ &+\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\frac{\partial A_S}{\partial t}\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)\\ =&\frac{i\hat{H}}{\hbar}\hat{A}_H(t)-\frac{i}{\hbar}A_H(t)\cdot\hat{H}\\ =&\frac{i}{\hbar}[\hat{H},\hat{A}_H(t)]+\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\frac{\partial A_S}{\partial t}\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)\end{aligned}$$

We the parallel between Schrodinger and Hamilton's equations, and Heisenberg's and Poisson's equation.

**Proposition.** Does the commutator relation $[\hat{x}(t),\hat{p}(t)] = i\hbar$ hold in Heisenberg's picture? We see that

$$\begin{aligned}\hat{x}(t)\hat{p}(t)-\hat{p}(t)\hat{x}(t) =&\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{x}\Big(-\frac{i\hat{H}t}{\hbar}\Big)\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{p}\Big(-\frac{i\hat{H}t}{\hbar}\Big)\\ &-\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{x}\Big(-\frac{i\hat{H}t}{\hbar}\Big)\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\hat{x}\Big(-\frac{i\hat{H}t}{\hbar}\Big)\\ =&\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)(\hat{x}\hat{p}-\hat{p}\hat{x})\Big(-\frac{i\hat{H}t}{\hbar}\Big)\\ =&i\hbar\end{aligned}$$

It is then important to check that $[\hat{a},\hat{a}^\dagger] = 1$ too!

## 21 Lecture 22 (May 26th)

**Remark.** Last class we have learned the time derivative of an operator in Heisenberg's picture, given by

$$\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}[\hat{H},\hat{A}_H(t)]+\exp\Big(\frac{i\hat{H}t}{\hbar}\Big)\frac{\partial\hat{A}_S}{\partial t}(t_{\mathrm{s}})\exp\Big(-\frac{i\hat{H}t}{\hbar}\Big)$$

The hamilotian in the Heisenberg picture is

$$\hat{H}_H = \exp\Big(\frac{i\hat{H}_St}{\hbar}\Big)\hat{H}_S\exp\Big(-\frac{i\hat{H}_St}{\hbar}\Big) = \hat{H}_S$$

from the fact that $[H^n,H] = H^nH - HH^n = 0$.

**Theorem.** (Harmonic oscillator) From $\hat{H}_S = \hbar\omega(\hat{a}^\dagger\hat{a}+1/2) = \hbar\omega(\hat{a}^\dagger(t)\hat{a}(t)+1/2) = \hat{H}_H$

we find

$$\begin{aligned}\frac{d\hat{a}(t)}{dt} =&\frac{i}{\hbar}[\hat{H},\hat{a}(t)] = i\omega[\hat{a}^\dagger(t)\hat{a}(t),\hat{a}(t)]\\ =&i\omega[\hat{a}^\dagger(t),\hat{a}(t)]\hat{a}(t) = -i\omega(t)\hat{a}(t)\end{aligned}$$

Solving the following the differential equation we find

$$\hat{a}(t) = e^{-i\omega t}\hat{a}(0)$$

Preforming the adjoint,

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

We can then seek (do this!) $\hat{x}(t)$ and $\hat{p}(t)$ and you will find dependence on $\hat{x}(0)$ and $\hat{p}(0)$ as if you solved the Newton's equations.

**Example.** Seek, for example,

$$\langle 0|\hat{a}(t)\hat{a}^\dagger(0)|0\rangle = e^{-i\omega t}\langle 0|\hat{a}(0)\hat{a}^\dagger(0)|0\rangle = e^{-i\omega t}$$

these functions are called correlation functions. Harmonic oscillators and angular momentum questions will be dealt in the final exam.

**Proposition.** Suppose you want to translate a wave function. Such a such that preforms this operation can be expressed as

$$\langle x|T(a)|\psi\rangle$$

where we want to move the wave function $a$ to the right.

$$\begin{aligned}\psi(x-a) =&\sum_{n=0}^{\infty}\frac{1}{n!}(-a)^n\frac{d^n}{dx^n}\psi(x) = \sum_{n=0}^{\infty}\frac{1}{n!}\Big(-\frac{ia}{\hbar}\Big)^n(-i\hbar)^n\frac{d^n}{dx^n}\psi(x)\\ =&\langle x|\sum_{n=0}^{\infty}\frac{1}{n!}\Big(-\frac{ia\hat{p}}{\hbar}\Big)^n|\psi\rangle = \langle x|\exp\Big(-\frac{ia\hat{p}}{\hbar}\Big)|\psi\rangle\end{aligned}$$

we thus find the translation operator to be a unitary operator

$$T(a) = \exp\Big(-\frac{ia\hat{p}}{\hbar}\Big)$$

**Definition.** (Angular momentum) Angular momentum is classically given as

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}$$

We find that

$$\begin{cases} L_x = yP_z - zP_y \\ L_y = zP_x - xP_z \\ L_z = xP_y - yP_x \end{cases}$$

Finding the comutators,

$$\begin{aligned}
[L_x, L_y] =& [yP_z - zP_y, zP_x - xP_z] \\
=& (yP_z - zP_y)(zP_x - xP_z) - (zP_x - xP_z)(yP_z - zP_y) \\
=& [yP_z, zP_x] - [yP_z, xP_z] - [zP_y, zP_x] + [zP_y, xP_z] \\
=& y[P_z, z]P_x - y[P_z, P_z]x - P_y[z, z]P_x + x[zP_y, P_z] + [zP_y, x]P_z \\
=& y(-i\hbar)P_x + x(i\hbar)P_y = i\hbar L_z
\end{aligned}$$

as

$$x[zP_y, P_z] + [zP_y, x]P_z = x(z[P_y, P_z] + (i\hbar)P_y)$$

Along this line,

$$[L_x, L_y] = i\hbar L_z \quad [L_y, L_z] = i\hbar L_x \quad [L_z, L_x] = i\hbar L_y$$

and we have

$$[L_a, L_b] = i\hbar \epsilon_{abc} L_c$$

with $(a, b, c) = (x, y, z)$. This forms a $SU(2)$ Lie algebra, and applies to spin also. Now take

$$\mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2$$

Finding the commutator with $L_z$,

$$[\mathbf{L} \cdot \mathbf{L}, L_z] = [L_x^2 + L_y^2, L_z] = [L_x^2, L_z] + [L_y^2, L_z] = 0$$

where

$$[L_x^2, L_z] = L_x[L_x, L_z] + [L_x, L_z]L_x = L_x(-i\hbar L_y) + (-i\hbar L_y)L_x$$

and

$$[L_y^2, L_z] = L_y[L_y, L_z] + [L_y, L_z]L_y = i\hbar L_y L_x + i\hbar L_x L_y$$

In quantum physics, we choose $\mathbf{L}^2$ and $L_z$ to be the commuting set with simulataneous eigenkets $|l, m\rangle$, which we define to satisfy the equations

$$\mathbf{L}^2 |l, m\rangle = \hbar^2 l(l+1) |l, m\rangle \quad \text{and} \quad L_z |l, m\rangle = \hbar m |l, m\rangle$$

From here, we see that

$$\langle l, m | \mathbf{L} \cdot \mathbf{L} | l, m\rangle = \hbar l(l+1) = \langle L_x lm | L_x lm\rangle + \ldots \geq 0$$

and we impose that $l \geq 0$. As $|l, m\rangle$ are eigenkets, we have

$$\langle l', m'|l, m\rangle = \delta_{ll'}\delta_{mm'}$$

These calculations are 1000% in the exams and must be memorised.

**Remark.** We now investigate

$$\begin{cases} L_+ = L_x + iL_y \\ L_- = L_x - iL_y \end{cases}$$

$[\mathbf{L}^2, L_\pm] = 0$ is trivial, meanwhile

$$[L_z, L_+] = \hbar L_+ \quad [L_z, L_-] = -\hbar L_-$$

## 22 Lecture 23 (May 28th)

**Recall.** Last time we have learned that

$$[L_i, L_j] = i\hbar\varepsilon_{ijk}L_k$$

and that for $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$ and $L_\pm = L_x \pm iL_y$, the following identities hold.

$$\begin{cases} [\mathbf{L}^2, L_a] = 0 & [L_z, L_+] = \hbar L_+ \\ [L_+, L_-] = 2\hbar L_z & [L_z, L_-] = -\hbar L_- \end{cases}$$

Also, we defined the simultaneous eigenvectors $|l, m\rangle$ to satifisfy

$$\mathbf{L}^2|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle \quad \text{and} \quad L_z|l, m\rangle = m\hbar|l, m\rangle$$

We notice that from $[\mathbf{L}^2, L_a] = 0$, we have $[\mathbf{L}^2, L_\pm] = 0$, or

$$\mathbf{L}^2(L_+|l, m\rangle) = L_+\mathbf{L}^2|l, m\rangle = l(l+1)\hbar^2(L_+|l, m\rangle)$$

Therefore, $L_+|l, m\rangle$ belongs to the $l$-multiplet. Continuing,

$$\begin{aligned} L_z(L_+|l, m\rangle) =& ([L_z, L_+] + L_+L_z)|l, m\rangle \\ =& (\hbar L_+ + m\hbar L_+)|l, m\rangle \\ =& (m+1)\hbar(L_+|l, m\rangle) \end{aligned}$$

From this we obtain the fact that

$$L_+|l, m\rangle = C_{lm}^+|l, m+1\rangle \quad \text{or} \quad L_-|l, m\rangle = C_{lm}^-|l, m-1\rangle$$

Taking the dual of the first,

$$\langle l, m|L_- = (C^+_{lm})^* \langle l, m+1|$$

Applying this to the ket $|l, m\rangle$,

$$\langle l, m|L_- L_+|l, m\rangle = |C^+_{lm}|^2 \langle l, m+1|l, m+1\rangle$$

The operator on the left is equal to $\mathbf{L}^2 - L_z^2 - \hbar L_z$. We then have

$$|C^+_{lm}|^2 = \hbar^2 (l-m)(l+m+1)$$

and further that

$$C^+_{lm} = \pm\hbar\sqrt{(l-m)(l+m+1)}$$

where we take the positive sign. On the other hand,

$$C^-_{lm} = \hbar\sqrt{(l+m)(l-m+1)}$$

you MUST do this. Now we have accumulated the following facts

$$\begin{cases} l \geq 0 \\ l(l+1) - m(m+1) \geq 0 \\ l(l+1) - m(m-1) \geq 0 \end{cases}$$

From this we obtain that

$$-l \leq m \leq l$$

which must be memorised. We lastly remark that operators like $\mathbf{L}^2$ are Casimir operators.

**Corollary.** We now have that

(i) $l \geq 0$

(ii) $-l \leq m \leq l$

(iii) $m$ has a minimum value $m_{\text{min}}$, abeit that it doesn't have to be $-l$

$$L_-|l, m_{\text{min}}\rangle = 0 = C^-_{l,m_{\text{min}}}|l, m_{\text{min}} - 1\rangle$$

which tells us that $C^-_{l,m_{\text{min}}} = 0$. In otherwords,

$$\sqrt{(l + m_{\text{min}})(l - m_{\text{min}} + 1)} = 0$$

which teaches us that $m_{\text{min}}$ is exactly $-l$. You should separately prove that identically, $m$ has a maximum of $m_{\text{max}} = +l$. Do this calculation.

(iv) $m$ has a maximum value $m_{\text{max}} = l$

(v) The possible values of $l$ values are given as $l \in \boldsymbol{Z} \cup \frac{1}{2}\boldsymbol{Z} \cup \{0\}$. We often write $l$ for integers, $s$ for fractional values, or $j$ altogether.

**Theorem.** Now we seek the matrix representation of these operators. Consider the following for $\langle l', m'|\hat{O}|l, m\rangle$:

(i) $\hat{O} = \mathbf{L}^2$, $l(l+1)\hbar\langle l', m'|l, m\rangle = l(l+1)\hbar^2\delta_{ll'}\delta_{mm'}$

(ii) $\hat{O} = L_z$, $m\hbar\delta_{ll'}\delta_{mm'}$

(iii) $\hat{O} = L_+$, $C^+_{lm}\delta_{ll'}\delta_{m'm+1}$ and therefore is not diagonal

**Definition.** (Conserved quantities) Consider, for $\partial\hat{O}_S/\partial t$, the Heisenberg equation

$$\frac{d\hat{O}_H}{dt} = \frac{i}{\hbar}[H, \hat{O}_H]$$

For $\hat{O}_H$ to be a conserved quantity,

$$\frac{d\hat{O}_S}{dt} = 0 \qquad \Longleftrightarrow \qquad [H, \hat{O}_H] = 0$$

**Theorem.** We found that the momentum operator was the generator of the unitary translational operator,

$$T(\mathbf{a}) = \exp\Big(-\frac{i\mathbf{p}\cdot\mathbf{a}}{\hbar}\Big)$$

with $T(\mathbf{a})|\mathbf{x}\rangle = |\mathbf{x}+\mathbf{a}\rangle$. Along this logic, what is the momentum operator $\mathbf{L}$ the generator of? We expect it to be rotation!

*Proof.* For a small rotation counter clock-wise,

$$\begin{cases} x' = x\cos\theta - y\sin\theta \approx x - y\theta \\ y' = x\sin\theta + y\cos\theta \approx x\theta + y \end{cases}$$

Then, the wave function can be expressed as

$$\begin{aligned}
\psi(x', y') =& \psi(x - y\theta, y + x\theta) \\
=& \psi(x, y) - y\theta\frac{\partial\psi}{\partial x} + x\theta\frac{\partial\psi}{\partial y} \\
=& \psi(x, y) - y\theta\Big(\frac{i}{\hbar}\Big)(-i\hbar)\frac{\partial\psi}{\partial x} + x\theta\Big(\frac{i}{\hbar}\Big)(-i\hbar)\frac{\partial\psi}{\partial y} \\
=& \frac{i\theta}{\hbar}\langle x, y|(-yP_x + xP_y)|\psi\rangle
\end{aligned}$$

We thus have found that the angular momentum operator is the generator of the unitary rotation operator.

$$U(\hat{n},\theta) = \exp\Big(-\frac{i\mathbf{J}\cdot\mathbf{n}\theta}{\hbar}\Big)$$

$\square$

## 23 Lecture 24 (June 2nd)

**Recall.** We have the following operators generating the time, translation, and rotation groups.

$$U_{\text{time}} = \exp\Big(-i\frac{Ht}{\hbar}\Big) \qquad U_{\text{tran}} = \exp\Big(-i\frac{\mathbf{p}\cdot\mathbf{a}}{\hbar}\Big) \qquad U_{\text{rot}} = \exp\Big(-i\frac{\mathbf{J}\cdot\mathbf{n}\,\theta}{\hbar}\Big)$$

**Proposition.** For the orbital angular momentum, we consider the transformation from cartesian to cylindrical coordinates

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}$$

with $(x,y,z)\to(r,\theta,\phi)$ through

$$\begin{cases} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{cases}$$

In the infinitesimal sense,

$$L_z = xP_y - yP_x = x\Big(i\hbar\frac{\partial}{\partial y}\Big) - y\Big(-i\hbar\frac{\partial}{\partial x}\Big) = -i\hbar\frac{\partial}{\partial\phi}$$

which should be calculated atleast once. By extension, we can also express $L_\pm$ in cartesian coordinates. Lastly, we can find $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$ to be

$$\mathbf{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

which is the Laplacian in terms of spherical coordinates.

**Theorem.** Memorize, again,

$$L_z|l,m\rangle = m\hbar|l,m\rangle \quad \text{and} \quad \mathbf{L}^2|l,m\rangle = l(l+1)\hbar^2|l,m\rangle$$

We define spherical harmonics as

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

We can write

$$\int d\mathbf{x}\,|\mathbf{x}\rangle\langle\mathbf{x}| = \mathbf{1} \quad \text{and} \quad \int d\Omega\,|\theta,\phi\rangle\langle\theta,\phi| = \mathbf{1}$$

Then,

$$\int \sin\theta d\theta d\phi\,|\theta,\phi\rangle\langle\theta,\phi|\theta',\phi'\rangle$$

We then require that

$$\langle\theta,\phi|\theta',\phi'\rangle = \frac{\delta(\theta-\theta')\delta(\phi-\phi')}{\sin\theta} = \delta(\cos\theta - \cos\theta')\delta(\phi-\phi')$$

We now seek

$$\langle\theta,\phi|\hat{L}_z|l,m\rangle = m\hbar\langle\theta,\phi|l,m\rangle$$

implying

$$-i\hbar\frac{\partial}{\partial\phi}\langle\theta,\phi|l,m\rangle = m\hbar\langle\theta,\phi|l,m\rangle$$

and

$$\frac{\partial}{\partial\phi}Y_{l,m}(\theta,\phi) = imY_{l,m}(\theta,\phi)$$

We now know that $Y_{l,m}(\theta,\phi) = e^{im\phi}F(\theta)/\sqrt{2\pi}$ with $m$ an integer, as the function should be periodic with respect to $\phi$. We now use the operator $\mathbf{L}^2$ to determine $F(\theta)$.

$$\langle\theta,\phi|\mathbf{L}^2|l,m\rangle = l(l+1)\hbar^2\langle\theta,\phi|l,m\rangle$$

We have

$$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\frac{e^{im\phi}}{\sqrt{2\pi}}F_{l,m}(\theta) = l(l+1)\hbar^2\frac{e^{im\phi}}{\sqrt{2\pi}}F_{l,m}(\theta)$$

and

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) - \frac{m^2}{\sin^2\theta}\right]F_{l,m}(\theta) = l(l+1)F_{l,m}(\theta)$$

This is the associated Legendre polynomial with $m \neq 0$ (Legendre if $m = 0$). Finite solutions with $0 \leq \theta \leq \pi$ require that $l \geq 0$ and $l \in \boldsymbol{Z}$.

$$F_{l,m}(\theta) = P_{l,m}(\cos\theta)$$

Substituting $z = \cos\theta$, we have the more famililar

$$\frac{d}{dz}\Big[(1-z^2)\frac{dP_{l,m}}{dz}\Big] + \Big[l(l+1) - \frac{m^2}{1-z^2}\Big]P_{l,m} = 0$$

with solutions

$$P_{l,m}(z) = (1-z^2)^{m/2}\frac{d^m}{dz^m}P_l$$

Normalisation can be done through setting

$$\langle l', m'|l, m\rangle = \delta_{ll'}\delta_{mm'}$$

We have, then,

$$\int d\Omega \langle l', m'|\theta, \phi\rangle\langle\theta, \phi|l, m\rangle = \int d\Omega\, Y^*_{l',m'}(\theta, \phi)Y_{l,m}(\theta, \phi) = \delta_{ll'}\delta_{mm'}$$

and set coefficients accordingly. Resultantly,

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

for $m \geq 0$ and

$$Y_{l,-m} = (-1)^m (Y_{l,m})^*$$

for $m < 0$.

**Corollary.** Consider

$$\sum_{l,m}\langle\theta', \phi'|l, m\rangle\langle l, m|\theta, \phi\rangle = \sum_{l,m} Y_{l,m}(\theta', \phi')Y^*_{l,m}(\theta, \phi) = \langle\theta', \phi'|\theta, \phi\rangle = \frac{\delta(\theta-\theta')\delta(\phi-\phi')}{\sin\theta}$$

this is called the closure relation.

**Definition.** The parity operator was defined as the operator that sends $\mathbf{x} \to -\mathbf{x}$. How does this work in spherical polar coordinates? We require that

$$\theta \to \pi - \theta \quad \text{and} \quad \phi \to \phi + \pi$$

This turns $\cos\theta \to -\cos\theta$, and to an extension,

$$Y_{l,m}(-\mathbf{n}) = (-1)^l Y_{l,m}(\mathbf{n})$$

under parity.

## 24 Lecture 25 (June 4th)

**Theorem.** In spherical polar coordinates, the Hamiltonian is given as

$$\hat{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}} + V(\mathbf{r})$$

The Laplacian in spherical coordinates is given as

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\underbrace{\left(\frac{\partial^2}{\partial \theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)}_{-\mathbf{L}^2/\hbar^2}$$

We want to solve

$$\hat{H}\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

When solving a problem in QM, we need to first find all operators that commute with the Hamiltonian. For a potential that only depends on the modulus of the distance $V(|\mathbf{r}|)$, we can compute the commutator

$$[\mathbf{p}^2, L_z] = [p_x^2 + p_y^2 + p_z^2, xp_y - yp_x] = 0$$

check this later on. On the otherhand, we can compute the following,

$$\begin{aligned}[L_z, V(|\mathbf{r}|)] =& [xP_y - yP_x, V(|\mathbf{r}|) = x[P_y, V(|\mathbf{r}|)] - y[P_x, V(|\mathbf{r}|)] \\ =& x(-i\hbar)V'(|\mathbf{r}|)\frac{y}{r} - y(-i\hbar)V'(|\mathbf{r}|)\frac{x}{r} = 0\end{aligned}$$

In sum,

$$[H, L_z] = 0 \quad \text{and} \quad [H, \mathbf{L}^2] = 0$$

and there exists simultaneous eigenfunctions of $H$ and $L_z$ and $\mathbf{L}^2$. We previously saw that $Y_{l,m}(\theta,\phi)$ is a set of eigenfunctions of $L_z$ and $\mathbf{L}^2$. We take the simultaneous eigenfunctions for the three operators to be $Y_{lm}(\theta,\phi)R_l(r)$. Under the assumption that we are dealing with eigenfunctions of the $\mathbf{L}^2$ operator, we have

$$\nabla \to \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}$$

and the full Schrodinger equation becomes

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + V(r) + \frac{l(l+1)\hbar^2}{2mr^2}\right]R_{nl}(r) = ER_{nl}(r)$$

**Remark.** (Solutions of the above formulation) Imagine solving the equation in the free-particle case, which we know the solution of to be $\exp(ip{\cdot}x)/(\sqrt{2\pi\hbar})^2$. With the substitution $\rho = kr$ and $k = 2mE/\hbar^2 > 0$, we have

$$\rho^2\frac{d^2R}{d\rho^2} + 2\rho\frac{dR}{d\rho} + (\rho^2 - l(l+1))R = 0$$

which is the spherical Bessel equation, an self-adjoint equation. Substitute $R(\rho) = Z(\rho)/\sqrt{\rho}$ to find

$$\rho^2 Z'' + \rho Z' + \left(\rho^2 - \left(l + \frac{1}{2}\right)^2\right)Z = 0$$

which is the original Bessel equations. The solutions are given as the Bessel functions $J_{l+1/2}(\rho)$ and the Neumann functions $N_{l+1/2}(\rho)$. Reserving the substitutions, we have the spherical Bessel and spherical Neumann functions $j_l(\rho)$ and $n_l(\rho)$. We can create linear combinations of these functions to obtain spherical Hankel functions, which represent travelling waves. In the limit, we have

$$j_l(\rho) \sim \frac{1}{\rho}\sin\Big(\rho - \frac{l\pi}{2}\Big) \quad n_l(\rho) \sim \frac{1}{\rho}\cos\Big(\rho - \frac{l\pi}{2}\Big)$$

**Example.** (Spherical well) Now consider the spherical well problem. When $r \geq a$, we have $R_l(r = a) = 0$. Inside the well, we have $j_l(kr)$ and $n_l(kr)$, but we reject the latter as $n_l(kr)$ diverges at the origin. As the wavefunction needs to be continuous at $r = a$, we have

$$j_l(ka) = 0$$

and $ka = x_{nl}$ where $x_{nl}$ denotes the $n$-th root of $j_l(x)$. We thus find $k$ to be $x_{nl}/a$ and the energy values to be

$$E_{nl} = \frac{\hbar^2}{2m}\Big(\frac{x_{nl}}{a}\Big)^2$$

The last step is normalisation. We impose that

$$\int_0^\infty r^2 dr\,(j_l)^2(Y_{lm})^2 = 1$$

to obtain the coefficients.

**Example.** (Hydrogen atom) For the Hydrogen atom, we need to substitute the Coulomb potential,

$$V(|\mathbf{r}|) = \frac{1}{4\pi\varepsilon_0}\frac{(-e)Ze}{r}$$

We note that we solve this for negative energy levels, we want bounded motion. Define $\rho = \sqrt{8m(-E)/\hbar^2}r$ and $\lambda = Z\alpha\sqrt{mc^2/2(-E)}$. We then have the equation

$$R'' + \frac{2}{\rho}R' - \frac{l(l+1)}{\rho^2}R + \Big(\frac{\lambda}{\rho} - \frac{1}{4}\Big)R = 0$$

We know that the asymptotic factor must be $\exp(-\rho/2)$, so we take the ansatz $R = \exp(-\rho/2)G(\rho)$ to find

$$G'' - \Big(1 - \frac{2}{\rho}\Big)G' + \Big[\frac{\lambda - 1}{\rho} - \frac{l(l+1)}{\rho^2}\Big]G = 0$$

As $\rho \to 0$, we find $G = \rho^l$ or $G = \rho^{-(l+1)}$. However, as $l \geq 0$, we take the prior, and again set yet another ansatz $R = \exp(-\rho/2)\rho^l H(\rho)$ to find

$$H'' + \Big(\frac{2l+1}{\rho} - 1\Big)H' + \frac{\lambda - l - 1}{\rho}H = 0$$

which follows the form of an Associated Laguerre equation. We can verify that for the Laguerre equations $L_{nr}^k$ satisfy

$$\rho(L_{n_r}^k)'' + (k+1-\rho)(L_{n_r}^k)' + n_r L_{n_r}^k = 0$$

## 25 Lecture 26 (June 9th)

**Remark.** Last class we have arrived at the differential equation

$$\rho H'' + (2l+2-\rho)H' + (\lambda - l - 1)H = 0$$

which followed the form of an associated Laguerre equation.

$$\rho(L_{n_r}^k)'' + (k+1-\rho)(L_{n_r}^k)' + n_r L_{n_r}^k = 0$$

Such a differential equation can be solved through the Frobenius method. We note that it is required that $n_r \in \boldsymbol{Z}^+$. We can equate the two equations with $k = 2l+1$ and $\lambda = n = l+1+n_r \geq 1$ ($n \in \boldsymbol{N}$). This $n$ is what we've learned in chemistry as the principle quantum number. With this information, we find the energy levels to be

$$E_n = -\frac{Z^2\alpha^2 mc^2}{2n^2} = -\frac{Z^2}{n^2}(13.6 \text{ eV})$$

In this equation, the mass $m$ is technically the reduced mass,

$$m = \frac{Zm_e m_p}{m_e + Zm_p}$$

The total wavefunction then becomes

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

For a particular $n$ and a corresponding energy level, there are $2n^2$ degeneracies, meaning that there are $2n^2$ states for a single energy level.

**Theorem.** (Separation of variables for the harmonic oscillator) Consider the Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V(x,y,z)$$

We sometimes take the potential to be a summation of component-dependent potentials $V(x,y,z) = V(x) + V(y) + V(z)$. Then, we can take $\psi(x,y,z) = X(x)Y(y)Z(z)$ as a separable solution. Also, take

$$V(x,y,z) = \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2 + \frac{1}{2}k_z z^2$$

and we can find the energy levels to be

$$\hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$$

Notice, how, we can also write the potential energy as $kr^2/2$. Then, we can also do variable separables and obtain a function in the form of

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$$

We notice how solutions can become very complex when using different coordinate systems.

**Definition.** We previously noted that the angular momentum can take half-integer values where we denote the values by $s$. Take $S = 1/2$, and we use the following conventions for the possible kets

$$\left|S = \frac{1}{2}, S_z = \frac{1}{2}\right\rangle = |\uparrow\rangle \qquad \left|S = \frac{1}{2}, S_z = -\frac{1}{2}\right\rangle = |\downarrow\rangle$$

We then see that $\langle\uparrow \mid \uparrow\rangle = \langle\downarrow \mid \downarrow\rangle = 1$ and $\langle\uparrow \mid \downarrow\rangle = 0$. With this information, we can find the matrix representation of $\hat{S}_z$ with respect to the above eigenkets that construct a basis, and we find

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z$$

The eigenkets are named qubits. We now define

$$S_\pm = S_x \pm iS_y$$

and seek their matrix representations. We find that

$$S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

from which follows that

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x \quad \text{and} \quad S_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y$$

The Pauli matrices together satisfy the following properties

(i) Hermitian

(ii) $\sigma_x^2 = \sigma_y^2 + \sigma_z^2 = I$ and hence unitary

(iii) $\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma k = -\sigma_j\sigma_i$ where $\{i, j, k\} = \{x, y, z\}$

(iv) $\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j - \sigma_j\sigma_i = \delta_{ij}2I$ which is to say that the Pauli matrices satisfy the Clifford algebra

## 26 Lecture 27 (June 11th)

**Theorem.** We try to seek the eigenvectors for $S_x$ and $S_y$ in the basis generated by $S_z$. The characteristic equation for $S_x$ is

$$\lambda^2 - \left(\frac{\hbar}{2}\right)^2 = 0$$

and $\lambda = \pm\hbar/2$. Let the first eigenvector be denoted as $v = (v_1, v_2)$ we find that $v_1 = v_2$ and from the normalisation condition, $v_1^2 + v_2^2 = 1$ and we find that $v_1 = v_2 = 1/\sqrt{2}$ where choose the sign to be positive by convention. We can also multiply $-1$ to either $v$ and $u$, but this would only change the spinor by a phase factor, and as same rays, they would have the same physical meaning.

$$v = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = |S_x, \uparrow\rangle \quad \text{and} \quad u = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = |S_x, \downarrow\rangle$$

for eigenvalues $\lambda_u = \hbar/2$ and $\lambda_v = -\hbar/2$ respectively. Similarly, the characteristic equation for $S_y$ is identical with $S_x$ and along with the normalisation condition, we find

$$v = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} = |S_y, \uparrow\rangle \quad \text{and} \quad u = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = |S_y, \downarrow\rangle$$

for eigenvalues $\lambda_v = \hbar/2$ and $\lambda_u = -\hbar/2$ respectively. We can additionally notice that they are perpendicular to each other.

**Proposition.** We now seek to the spin in an arbitrary direction $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the characteristic equation is still $\lambda^2 = n_x^2 + n_y^2 + n_z^2 = 1$. The problem set related to this will definitely be in the test!

**Remark.** Consider an arbitrary spin state that is normalised. What is the probability that the result is $-\hbar/2$ when it is measured in the $\hat{n}$ direction? We simply expand the state with respect the basis and calculate the square of the coefficients.

$$|\psi\rangle = c_1|\mathbf{S}\cdot\hat{n}, \uparrow\rangle + c_2|\mathbf{S}\cdot\hat{n}, \downarrow\rangle$$

**Theorem.** We show that there exists an operator that changes the spin state by an angle $\phi$.

$$\exp\left(-\frac{i\mathbf{S}\cdot\hat{n}\,\phi}{\hbar}\right)$$

For simplicity, take $\hat{n} = \hat{\mathbf{x}}$.

$$\exp\Big(-\frac{i\sigma_x\phi}{2}\Big) = \sum_{n\in 2\boldsymbol{Z}} \frac{1}{n!}\Big(-\frac{i\phi}{2}\Big)^n (\sigma_x)^n + \sum_{n\in 2\boldsymbol{Z}+1} \Big(-\frac{i\phi}{2}\Big)^n (\sigma_x)^n$$

Which equal to

$$\cos\Big(\frac{\phi}{2}\Big)I - i\sin\Big(\frac{\phi}{2}\Big)\sigma_x = \begin{pmatrix} \cos\frac{\phi}{2} & -i\sin\frac{\phi}{2} \\ -i\sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix}$$

Lets take the $(1,0)$ ket and rotate it by using the above matrix with $\phi = \pi/2$. What we expect is it to lie in $S_y$. This is true as we find

$$U_{\pi/2}(\hat{\mathbf{x}}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

We can caluclate to also find that after 360 degrees, the matrix is

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

and after 720 degrees, the matrix is

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

In this sense, spinors are double valued.

**Remark.** There exists (god given) magnetic moment for electrons. To properly approach this, we require the Dirac equation, where we would apply an operator to the equation and do unrelativistic approximations. We then find

$$\hat{\mathbf{H}} = -\boldsymbol{\mu}\cdot\mathbf{B}(t)$$

with

$$\boldsymbol{\mu} = \frac{q(-e)}{2m_e}\mathbf{S}$$

and $g = 2\times 1.0011596\ldots$. For orbital angular momentum, $g = 1$. Let try and use this Hamiltonian to solve the equations of motion. What we expect is precessional motion.

*Proof.* Take

$$|\psi(t)\rangle = \begin{pmatrix} \alpha_\uparrow(t) \\ \alpha_\downarrow(t) \end{pmatrix}$$

and we have

$$\frac{eg\hbar}{4m_e}\boldsymbol{\sigma}\cdot\mathbf{B}(t)\begin{pmatrix} \alpha_\uparrow(t) \\ \alpha_\downarrow(t) \end{pmatrix} = i\hbar\begin{pmatrix} \dot{\alpha}_\uparrow(t) \\ \dot{\alpha}_\downarrow(t) \end{pmatrix}$$

Taking $\mathbf{B} = B_0\hat{\mathbf{z}}$, we simply have the differential equations

$$i\dot{\alpha}_\uparrow(t) = \frac{egB_0}{4m_e}\alpha_\uparrow(t)$$

and

$$i\dot{\alpha}_\downarrow(t) = -\frac{egB_0}{4m_e}\alpha_\downarrow(t)$$

These have simple solutions,

$$\begin{cases} \alpha_\uparrow(t) = \alpha_\uparrow(0)e^{-iw_0t} \\ \alpha_\downarrow(t) = \alpha_\downarrow(0)e^{iw_0t} \end{cases}$$

Finding the expectation values with assuming hat initially the spin was up with $\alpha_\uparrow(0) = \alpha_\downarrow(0) = 1/\sqrt{2}$, we have

$$\langle\psi(t)|\hat{S}_x|\psi(t)\rangle = \frac{\hbar}{2}\frac{1}{\sqrt{2}}(e^{i\omega_0t}, e^{-i\omega_0t})\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\omega_0t}\\ e^{i\omega t}\end{pmatrix} = \frac{\hbar}{4}(e^{2i\omega_0t}+e^{-2i\omega_0t}) = \frac{\hbar}{2}\cos(2\omega_0t)$$

for $S_y$, we find the same result but with the sine function. □

## 27 Lecture 28 (June 16th)

**Theorem.** (Addition of angular momentum) The sum of two angular momentum operators

$$\mathbf{J} = \mathbf{J}_1 \otimes I_2 + I_1 \otimes \mathbf{J}_2$$

must operate both on $|j_2, j_{1z}\rangle$ (the Hilbert space generated by $\mathbf{J}_1$) and $|j_2, j_{2z}$, and therefore acts on the tensor product $|j_1, j_{1z}\rangle \otimes |j_2, j_{2z}\rangle = |j_1, j_{1z}; j_2, j_{2z}$. Note that $[J_{1a}, J_{2b}] = 0$ and that

$$\mathbf{J}^2|j, j_z\rangle = \hbar^2 j(j+1)|j, j_z\rangle$$

with

$$\mathbf{J}_z|j, j_z\rangle = j_z\hbar|j, j_z\rangle$$

We naively take the maximum to be $j_{max} = j_1 + j_2$ and $j_{min} = |j_1 - j_2|$. We now try adding two $S = 1/2$ (Important). We define the total spin as

$$\mathbf{S} = \mathbf{S}_1 \otimes I_2 + I_1 \otimes \mathbf{S}_2$$

with $\mathbf{S}_1$ acting on elements such as $|S_1 = 1/2, S_{1,z}\rangle$ and $\mathbf{S}_2$ acting on elements such as $|S_2 = 1/2, S_{2,z}\rangle$. Then, $\mathbf{S}$ acts on

$$\left|S_1 = \frac{1}{2}, S_{1,z}\right\rangle \otimes \left|S_2 = \frac{1}{2}, S_{1,z}\right\rangle = |S_{1,z}, S_{2,z}\rangle$$

Trying to find the basis of $\mathbf{S}$ starting with $s = 1$ (triplet) we find

$$|s = 1, s_z = 1\rangle = |1/2, 1/2\rangle \otimes |1/2, 1/2\rangle$$

and

$$|s - 1, s_z = -1\rangle = | - 1/2, -1/2\rangle$$

what about the middle state with spin 1? We apply $S_- = S_{1,-} + S_{2,-}$ and find

$$|s = 1, s_z = 0\rangle = \frac{1}{\sqrt{2}}\Big(\Big|\frac{1}{2}, -\frac{1}{2}\Big\rangle + \Big| - \frac{1}{2}, \frac{1}{2}\Big\rangle\Big)$$

Now we move on to $S = 0$, where the total spin is 0. We know its going to be a linear combination of $|\uparrow,\downarrow\rangle$ and $|\downarrow,\uparrow\rangle$. As it should be perpendicular with $|1, 0\rangle$, we find

$$|S = 0, S_z = 0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\Big)$$

Does this truely have zero spin ($S = 0$)? Applying $\mathbf{S}^2$ we find

$$\mathbf{S}^2\frac{1}{\sqrt{2}}\Big(\Big|\frac{1}{2}, -\frac{1}{2}\Big\rangle - \Big| - \frac{1}{2}, \frac{1}{2}\Big\rangle\Big)$$

and using

$$\mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2 + S_z^2 = \frac{1}{2}(S_+S_- + S_-S_+) + S_{1z}^2 + S_{2z}^2 + 2S_{1z}S_{2z}$$

we conclude from

$$\frac{1}{2}S_+S_-(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{1}{2}S_+(|\downarrow\downarrow\rangle - |\downarrow\downarrow\rangle) = 0$$

by the same argument, $S_-S_+|0, 0\rangle = 0$ and the remaining calculations on $S_z^2$ also dissapear. We thus see how indeed, the postulated vector has a spin of zero. Is the singlet separable? That is, is

$$|S = 0, S_z = 0\rangle = (a|\uparrow\rangle_1 + b|\downarrow\rangle_1) \otimes (c|\uparrow\rangle_2 + d|\downarrow\rangle_2)$$

we find through algebra that either $ac = bd = 0$, and additionally that there is no solution to these equations. Therefore, we find that that certain state is entangled.