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 ψ, 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 ($\Delta x \Delta p \geq i\hbar$).

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 $A(k)$.

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

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

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

with the weight function (Fourier transform) given by

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

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 $(\mathit{\Delta} k/2)^2 = \alpha$ and $\mathit{\Delta} k = 2\sqrt{\alpha}$.

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,

$$\oint_C dz\ f(z) = 0$$

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 β 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 $2\sqrt{(\alpha^2+\beta^2t^2)/\alpha}$, 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 ψ_1 and the electron going through the second slit would be expressed as ψ_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:

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

Proof. Note that

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

We then have

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

From here, we impose that the last term, which we define as the probability current (technically negative of this value), to be equal to zero, which allows the probability interpretation to be valid. This is a boundary condition for the wavefunction to follow that we mentioned above. In multiple dimensions,

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

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

$$-\frac{\hbar}{2im}\int_{\partial V}\mathbf{j}\cdot d\mathbf{a} = 0$$

$\square$

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

Definition. (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

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

Theorem. (Ehrenfest theorem) We derive that the expectation value interpretation is valid by verifying that

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

Proof. By using the Schrodinger equation and integration by parts twice,

$$\begin{aligned}
m\frac{d}{dt}\langle x\rangle =& m\frac{d}{dt}\int dx\ \Psi^* x\Psi \\
=& m\int dx\ x\frac{\partial \Psi^*}{\partial t}\Psi + x\Psi^*\frac{\partial \Psi}{\partial t} \\
=& m\int dx\ x\Big(\frac{\hbar}{2im}\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\hbar}{2im}\frac{\partial^2\Psi}{\partial x^2}\Big) \\
=& -\frac{i\hbar}{2}\Big[x\Psi\frac{\partial\Psi}{\partial x}\Big|_a^b + \int dx\ -\frac{\partial\Psi^*}{\partial x}\Big(\Psi + x\frac{\partial\Psi}{\partial x}\Big) - \Psi^*\frac{\partial^2\Psi}{\partial x^2}x\Big] \\
=& -\frac{i\hbar}{2}\Big[x\Psi\frac{\partial\Psi}{\partial x}\Big|_a^b - \Big(\Psi + x\frac{\partial\Psi}{\partial x}\Big)\Psi^*\Big|_a^b + \int dx\ \Psi^*\Big(2\frac{\partial\Psi}{\partial x} + x\frac{\partial^2\Psi}{\partial x^2}\Big) - \Psi^*\frac{\partial^2\Psi}{\partial x^2}x\Big] \\
=& -i\hbar\int dx\ \Psi^*\frac{\partial}{\partial x}\Psi + (\text{boundary terms})
\end{aligned}$$

□

Definition. (Canonical commutator relation for position and momentum) What is the observable is a polynomial expression of x and p? See that

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

We have therefore proven the following commutator relation:

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

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

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

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

for physical measurements to make sense. An equivalent statement is that $\hat{A}$ 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 ($\hat{H}$) is also.

Theorem. (Parseval's theorem) The Fourier transformation preserves the integral of the square of the function. Here, we prove it specifically for wave packets and their Fourier transform.

$$\begin{aligned}
1 = \int_{-\infty}^{\infty} dx\ |\Psi(x)|^2 &= \int_{-\infty}^{\infty} dx\ \Psi^*(x)\Psi(x) \\
&= \int_{-\infty}^{\infty} dx\ \Big(\int_{-\infty}^{\infty} \frac{dp'}{\sqrt{2\pi\hbar}}\ \phi^*(p')e^{-ip'x/\hbar}\Big)\Big(\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}}\ \phi(p)e^{ipx/\hbar}\Big) \\
&= \int_{-\infty}^{\infty} dx\ \int_{-\infty}^{\infty} \frac{dp'}{\sqrt{2\pi\hbar}}\Big(\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}}\ \phi^*(p')\phi(p)e^{i(p-p')x/\hbar}\Big) \\
&= \int_{-\infty}^{\infty} dp\ |\phi(p)|^2
\end{aligned}$$

In the last line we have used Fubini's theorem and

$$\int_{-\infty}^{\infty} dx\ e^{-i(p-p')x/\hbar} = 2\pi\hbar\delta(p-p')$$

Parseval's theorem tells us that if the wave function in the position space is squared-integrable, the function in the momentum space also is.

Theorem. (Momentum operator in the momentum space) We have previously saw that the position operator in the position space was simply definition by multiplication. We can also ask, then, what the momentum operator is in the momentum space.

$$\langle p\rangle = \int_{-\infty}^{\infty} \Psi^* \cdot -i\hbar\frac{\partial}{\partial x}\Psi = \int_{-\infty}^{\infty} dx\ \Big(\frac{dp}{\sqrt{2\pi\hbar}}\ \phi^*(p)e^{-ipx/\hbar}\Big)\cdot -i\hbar\Big(\int_{-\infty}^{\infty} \frac{dp'}{\sqrt{2\pi\hbar}}\ \phi(p')\frac{ip}{\hbar}e^{ip'x/\hbar}\Big)$$

which becomes

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

7 Lecture 7 (March 26th)

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?

$$\begin{aligned}
\langle x\rangle =& \int dx\,\Big(\int_{-\infty}^{\infty}\frac{dp}{\sqrt{2\pi\hbar}}\;\phi^*(p)e^{-ipx/\hbar}\Big)x\Big(\int_{-\infty}^{\infty}\frac{dp'}{\sqrt{2\pi\hbar}}\;\phi(p')e^{ip'x/\hbar}\Big)\\
=&\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp\int_{-\infty}^{\infty}dp'\Big(\int_{-\infty}^{\infty}dx\;\phi^*(p)\phi(p')\cdot -i\hbar\frac{\partial}{\partial p'}e^{ix(p'-p)/\hbar}\Big)\\
=&\int_{-\infty}^{\infty}dp\int_{-\infty}^{\infty}dp'\;\phi^*(p)\phi(p')\cdot -i\hbar\frac{\partial}{\partial p'}\delta(p'-p)\\
=&\int_{-\infty}^{\infty}dp\int_{-\infty}^{\infty}dp'\;\phi^*(p)\cdot i\hbar\frac{\partial}{\partial p'}\phi(p')\delta(p'-p)\\
=&\int_{-\infty}^{\infty}dp\;\phi^* i\hbar\frac{\partial}{\partial p}\phi(p)
\end{aligned}$$

Definition. 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) $\langle v, a_1w_1+a_2w_2\rangle = a_1\langle v,w_1\rangle + a_2\langle v,w_2\rangle$ (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

$$L(a_1v_1+a_2v_2) = a_1L(v_1)+a_2L(v_2)$$

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 understand 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 vanishes at the endpoints and beyond. 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 span 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) Eigenvectors (functions) are orthogonal

(iii) The vector space spanned by the eigenvectors (functions) are complete

9 Lecture 9 (April 2nd)

Definition. (Parity transformation) 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

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

As the parity operator is involutive, it has eigenvalues $\lambda^2 = 1$. Therefore, we deduce that it can have even and odd functions as eigenfunctions. In the case of the potential well problem, setting our origin to $x = a/2$, we now have two operators and two corresponding eigenvalues,

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

Theorem. (Commutator relation for the Hamiltonian and parity) As the wavefunctions are simutaneously satisfy the eigenfunctions of $\hat{H}$ and $\mathcal{P}$, we now derive that $[\hat{H}, \mathcal{P}] = 0$ for symmetric potential functions ($V(x) = V(-x)$).

Proof. Observe that the below vanishes if $V(x) = V(-x)$.

$$\begin{aligned}
[\hat{H}, \mathcal{P}]\psi(x) =& \hat{H}\mathcal{P}\psi(x) - \mathcal{P}\hat{H}\psi(x) \\
=& \hat{H}\psi(-x) - \mathcal{P}\Big(- \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x)\Big) \\
=& \Big(- \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(-x) + V(x)\psi(-x)\Big) - \Big(- \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(-x) + V(-x)\psi(-x)\Big)
\end{aligned}$$

□

Theorem. (Commutator relation for the parity and momentum) What about $\hat{P}$ and $\hat{p}$?

$$\begin{aligned}
[\mathcal{P}, \hat{p}]\psi =& \mathcal{P} \cdot -i\hbar\frac{\partial\psi(x)}{\partial x} - \hat{p}\psi(-x) \\
=& -i\hbar\frac{\partial\psi(-x)}{\partial(-x)} + i\hbar\frac{\partial\psi(-x)}{\partial x} \\
=& -2\hat{p}\mathcal{P}\psi(x)
\end{aligned}$$

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

Theorem. (Interpretation of eigenvector coefficients) 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 eigenvectors would be shared and corresponding eigenvalues would come out.

Example. (Box quantisation) We observe how momentum can be quantised through imposing periodic boundary conditions. For the momentum operator, we previously looked at the following complex plane wave solution:

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

Calculating the inner product between two plane waves with different momentum we have

$$\langle\psi_{p'} \mid \psi_p\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\ \psi^*_{p'}(x)\psi_p(x) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\ \exp\Big(\frac{i(p-p')x}{\hbar}\Big) = \delta(p-p')$$

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

$$\exp\left(\frac{ipL}{\hbar}\right) = 1 \quad \rightarrow \quad p_n = \frac{2\pi n\hbar}{L}$$

for $n \in \boldsymbol{Z}$. In addition, taking $|\psi_p| = c$, for $p = p'$,

$$\langle \psi_{p'} \mid \psi_p \rangle = Lc^2 = 1$$

and obtain the condition $c = 1/\sqrt{L}$. In sum, box quantisation has two roles: (1) quantising physical quantities and (2) making inner products finite.

Example. For a wave function given a cyclic boundary condition $\phi(x) = \phi(x+L)$ on $[-L/2, L/2]$, its Fourier expansion would be given as

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

with coefficients

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

10 Lecture 10 (April 7th)

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 step functions, wells, barriers, delta functions, and simple harmonic oscillators.

Theorem. (Step function) Let us consider the step function potential given by:

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

Proof. $(E > V_0)$ For each region, we have the ansatz

$$\begin{cases} \psi_I(x) = e^{ikx} + Re^{-ikx} & x < 0 \\ \psi_{II}(x) = Te^{iqx} & 0 \le x \end{cases}$$

with $k^2 = 2mE/\hbar^2$ and $q^2 = 2m(E - V_0)/\hbar$. We impose two boundary conditions,

(i) (continuity at zero) $\psi_I(0) = \psi_{II}(0)$

(ii) (derivative continuity at zero) $\psi_I'(0) = \psi_{II}'(0)$

We have the following simultaneous equations as the result

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

with solutions

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

As a tangential remark, we note that using the definition of current density as density times velocity gives an equivalent equation, namely

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

□

Proof. ($E < V_0$) For each region, we have the same ansatz for region I, but in region II, we only take the negative exponential for normalisability. Imposing the boundary conditions we have the following simultaneous equations

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

with solutions

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

Notice that $R^2 = 1$ whereas the transmission coefficent doesn't vanish. □

11 Lecture 11 (April 9th)

Theorem. (Potential well) Let us consider the well potential given by:

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

Proof. ($E < -V_0$) No solutions exist, as continuity cannot be met. □

Proof. ($0 < E$) The scattering state (unbounded state) solutions have the initial ansatz

$$\begin{cases} \psi_I(x) = e^{ikx} + Re^{-ikx} & x < -a \\ \psi_{II}(x) = Ae^{iqx} + Be^{-iqx} & -a < x < a \\ \psi_{III}(x) = Te^{ikx} & a < x \end{cases}$$

with $k^2 = 2mE/\hbar^2$ and $q^2 = 2m(E + V_0)/\hbar^2$. We impose two boundary conditions,

(i) (continuity of logarithm) At $-a$ and a, the following is continuous.

$$\frac{1}{\psi}\frac{\partial\psi}{\partial x} = \frac{\partial}{\partial x}(\ln\psi)$$

(ii) (continuity of probability current density) $j_I(-a) = j_{II}(-a)$ and $J_{II}(a) = J_{III}(a)$

We have the following simultaneous equations as the result

$$\begin{aligned} \frac{\hbar k}{m}(1 - R^2) =& \frac{\hbar q}{m}(A^2 - B^2) = \frac{\hbar k}{m}T^2 \\ \frac{iqAe^{-iqa} - iqBe^{iqa}}{Ae^{-iqa} + Be^{iqa}} =& \frac{ike^{-ika} - ikRe^{ika}}{e^{-ika} + Re^{ika}} \\ \frac{iqAe^{iqa} - iqBe^{-iqa}}{Ae^{iqa} + Be^{-iqa}} =& \frac{ikTe^{ika}}{Te^{ika}} = ik \end{aligned}$$

with solutions

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

The numerator of R contains a sine function $\sin 2qa$. This means that $R = 0$ when:

$$\sin 2qa = 0 \quad \Rightarrow \quad 2qa = n\pi \quad \text{for } n \in \mathbb{Z}.$$

So at certain discrete values of energy (since q depends on energy), the reflection coefficient vanishes — that is, the particle is fully transmitted through the barrier. This phenomena has been well studied, for example, as a Ramsauer–Townsend resonance. $\square$

Theorem. (Barrier problem) Let us consider the barrier potential given by:

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

Proof. For each region, we have the ansatz

$$\begin{cases} \psi_I(x) = e^{ikx} + R^{-ikx} & x < -a \\ \psi_{II}(x) = Ae^{-qx} + Be^{qx} & -a < x < a \\ \psi_{III}(x) = Te^{ikx} & a < x \end{cases}$$

with $q^2 = 2m(V_0 - E)/\hbar$. We impose two boundary conditions and get the following simultaneous equations as the result

(i) (continuity at $-a$) $e^{-ka} + Re^{ika} = Ae^{qa} + Be^{-qa}$

(ii) (continuity at a) $Ae^{-qa} + Be^{qa} = Te^{ika}$

(iii) (derivative continuity at $-a$) $ike^{-ika} - ikRe^{ika} = -qAe^{qa} + Bqe^{-qa}$

(iv) (derivative continuity at a) $-qAe^{-qa} + qBe^{qa} = ikTe^{ika}$

with solutions

$$\begin{cases} T^2 = \dfrac{(2kq)^2}{(2kq)^2\cosh^2(2qa) + (k^2 - q^2)^2\sinh^2(2qa)} \\ R^2 = \dfrac{(k^2 + q^2)\sinh^2(2qa)}{(2kq)^2 + (k^2 + q^2)^2\sinh^2(2qa)} \end{cases}$$

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

$$\begin{aligned} j(x) =& \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right) \\ =& \frac{\hbar}{2im} 2q(-AB^* + A^*B) = \frac{\hbar k}{m} T^2 \end{aligned}$$

When x is larger than 1, we can approximate $\sinh x \sim e^x/2$ and we can approximate

$$T^2 \sim Ce^{-2(2qa)}$$

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

$$T^2 \sim \exp\Big[-2\int_{x_1}^{x_2} dx\,\sqrt{\frac{2m}{\hbar^2}(V(x)-E)}\Big]$$

$\square$

12 Lecture 12 (April 14th)

Example. Consider a metal apparatus where an electric field of magnitude E is applied. The potential energy of an electron given by the field is given as by $V(x) = W - (Ee)x$ where W is the work-function of the metal. Then,

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

with $W/eE = a$. This equation is called the Fowler-Nordheim equation.

Theorem. (Potential well) Let us again consider the well potential given by:

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

Proof. ($-V_0 < E < 0$) The bounded state solutions have the initial ansatz

$$\begin{cases} \psi_I(x) = Ae^{\alpha x} & x < -a \\ \psi_{II}(x) = B\cos kx + C\sin kx & -a < x < a \\ \psi_{III}(x) = Ae^{-\alpha x} & a < x \end{cases}$$

We impose two boundary conditions and get the following equations as the result

(i) (continuity of ψ'/ψ for the even parity)

$$\frac{-k\tan ka}{\alpha} = 1$$

(ii) (continuity of ψ'/ψ) for the odd parity)

$$\frac{k\cot ka}{\alpha} = -1$$

with solutions

$$\begin{cases} \text{even parity :} & \dfrac{\sqrt{\lambda - y^2}}{y} = \tan y \\ \text{odd parity :} & \dfrac{\sqrt{\lambda - y^2}}{y} = -\cot y \end{cases}$$

with dimensionless quantities

$$y = qa \qquad \lambda = \frac{2mV_0a^2}{\hbar^2}$$

We notice that the deeper and/or broader the potential well is (λ is bigger), there are more bound states that can be occupied. In addition, we find that odd and even eigenfunctions have inherently different energy levels, and that asymmetrical eigenfunctions therefore cannot exist. □

13 Lecture 13 (April 16th)

Remark. In a double potential well, the superposition of the two eigenfunctions ($\psi_e - \psi_o$ or $\psi_e + \psi_o$) gives an asymmetrical distribution. Let's say that the wave function is initially in the right:

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

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. (Dirac function potential) Let us consider the Dirac function potential

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

where λ is a dimensionless constant.

Proof. The Schrodinger equation is

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

and we have the initial ansatz

$$\begin{cases} \psi_I(x) = c_1 e^{-\kappa x} & x < 0 \\ \psi_{II}(x) = c_2 e^{\kappa x} & 0 < x \end{cases}$$

with $-\kappa^2 = 2mE/\hbar$. We impose the following boundary conditions

(i) (continuity at $x = 0$) We discover that $c_1 = c_2 = c$.

(ii) (derivative continuity at 0) From which we get

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

leading to

$$\begin{aligned} \psi'_{II}(0) - \psi'_I(0) =& \frac{\lambda}{a}\psi(0) \\ c(-\kappa) - c(\kappa) =& -c\frac{\lambda}{a} \end{aligned}$$

with a single solution $2\kappa = \lambda/a$. 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)! ☐

Theorem. (Harmonic oscillator) Let us consider the harmonic oscillator potential given by:

$$V(x) = \frac{1}{2}m\omega^2 x^2$$

Proof. The Schrodinger equation is

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

Substitute dimensionless constants $\varepsilon = 2E/\hbar\omega$ and $y = \sqrt{m\omega^2 x^2/\hbar^2}$. Then,

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

We set $\psi(y) = h(y)e^{-y^2}$ and find

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

Notice that this is a Hermite differential equation, solvable using the Frobenius method.

Likewise, we substitute the following idicial equation centered at $y = 0$:

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

obtaining

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

$j = 0, 1$ have no matching indexes, and we are able to consider these separately to arrive at an indicial equations

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

Back to Hermite differential equation, we set $j' = j - 2$ to obtain

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

We now arrive at a recurrence equation,

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

$\square$

14 Lecture 14 (April 21st)

Proof. Let's attempt to get a complete solution. We see from the indicial equation we can either take $k = 0, 1$.

$$\begin{aligned}
a_2 =& \frac{2(0-(\varepsilon-1)/2)}{2!}a_0 && (k=0) \\
a_4 =& \frac{2^2(2-(\varepsilon-1)/2)(0-(\varepsilon-1)/2}{4!}a_0 && (k=0) \\
a_2 =& \frac{2(1-(\varepsilon-1)/2)}{3!}a_0 && (k=1) \\
a_4 =& \frac{2^2(3-(\varepsilon-1)/2)(1-(\varepsilon-1)/2)}{5!}a_0 && (k=1)
\end{aligned}$$

For a generic ε, the series isn't terminated, and we need truncation. We find that we require $(\varepsilon - 1)/2 \in \boldsymbol{Z}^+$ and that

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

$\square$

Example. From the above, it is quite obvious that $n \in 2\boldsymbol{Z}$ denote even solutions while $n \in 2\boldsymbol{Z}+1$ denote odd solutions. Finding a few solutions we have (we used the normalisation condition for the coefficents): ...

Theorem. (Orthogonality of $\psi_n(x)$) Let ψ_i and ψ_j be two different wave function solutions of the form

$$\psi_n(x) = N_n H_n(y) e^{-y^2/2}, \quad \text{where} \quad \xi = \sqrt{\frac{m\omega}{\hbar}}x$$

We then subtract the following two expressions

$$\begin{aligned} \psi_i'' \psi_j^* &= -\frac{mk}{\hbar^2}x^2 \psi_i \psi_j^* - \frac{2mE_i}{\hbar^2}\psi_i \psi_j^* \\ (\psi_j^*)'' \psi_i &= -\frac{mk}{\hbar^2}x^2 \psi_j^* \psi_i - \frac{2mE_j}{\hbar}\psi_j^* \psi_i \end{aligned}$$