Quantum Mechanics I

Telmo Cunha

December 2025

Abstract

This is a set of notes (**in progress**) following a series of lectures on quantum mechanics, "Quantum Mechanics I" by Prof. Barton Zwiebach from MIT OpenCourseWare. The course can be found here. The main textbook used is [GS18].

Contents

1 Basic Concepts

1.1 Linearity

The idea of superposition in physics is essentially captured by the concept of a linear operator.

Definition 1.1. ***(Linear Operator)***
Suppose u, v solves $Lu = 0$, $Lv = 0$. We say that L is a linear operator if

$$\begin{aligned} L(\alpha u) &= \alpha L(u) = 0, \\ L(u+v) &= L(u) + L(v) = 0, \end{aligned} \tag{1.1}$$

for $\alpha \in \mathbb{R}$.

Maxwell's equations are linear equations while, in most cases of interest, Newton's equation is not. Consider

$$m\frac{d^2x(t)}{dt^2} = -V'(x(t)), \tag{1.2}$$

which is usually nonlinear depending on V'.
Quantum mechanics is a linear theory, Schrödinger's equation is given by

$$i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi, \tag{1.3}$$

where $\hat{H}$, the Hamiltonian, is a linear operator.

1.2 Complex Numbers

Useful identities about complex numbers.

$$z = a + ib, \quad a, b \in \mathbb{R}. \tag{1.4}$$

$$\bar{z} = a - ib, \quad a, b \in \mathbb{R}. \tag{1.5}$$

$$\|z\| = \sqrt{a^2 + b^2}. \tag{1.6}$$

$$\|z\|^2 = a^2 + b^2 = z\bar{z}. \tag{1.7}$$

Proposition 1.1.

$$z = \cos\theta + i\sin\theta = e^{i\theta}. \tag{1.8}$$

Proof. ... ■

The wave function $\Psi \in \mathbb{C}$ and $\|\Psi\|^2$ is interpreted as a probability.

1.3 Determinism

Photon energy is given by

$$E = h\nu, \tag{1.9}$$

where ν satisfies

$$\nu\lambda = c, \tag{1.10}$$

λ the wavelength and c the speed of light.

Polarizer experiment: if every photon in a beam of light is identical and that beam of light passes through a polarizer which is polarized along a direction of angle α with respect to the $x-$axis, then photons pass along the $x-$axis with probability $cos^2(\alpha)$ and get absorbed by the polarizer with probability $sin^2(\alpha)$. This is a deeply non-classical result, i.e. non-deterministic.

End of Lecture 1

1.4 Nature of Superposition in Quantum Mechanics

Mach-Zehnder Interferometer: Each individual photon is in a superposition, simultaneously in the upper beam and the lower beam, and interferes with itself.

If we have a superposition $|\Psi\rangle = \alpha\,|A\rangle + \beta\,|B\rangle$, any measurement of $|\Psi\rangle$ returns either a or b, if when measuring $|A\rangle$ you get a and when measuring $|B\rangle$ one gets b. The probability of measuring a is proportional to $\|\alpha\|^2$ while the probability of measuring b is proportional to $\|\beta\|^2$. After measurement the wave function collapses to the measured state.

Remark 1.1. *There are experiments which show that ensembles of particles with spin* $1/2$ *actually live in a superposition of states with spin up and spin down as oppose to an ensemble of particles where half have spin up and half have spin down. See the discussion at the end of lecture 6.*

Entanglement: For two particles, a state which can not be factorized as a tensor product of two distinct states is called an entangled state. For example

$$|u_1\rangle \otimes |v_1\rangle + |u_2\rangle \otimes |v_2\rangle \neq (...)_1 \otimes (...)_2\,. \tag{1.11}$$

Once we measure the state of one particle, the other is automatically known. Apparently this can work with entangled particles at distances of ate least 100km. (Look at Bell inequalities eventually!)

(really cool idea) Elitzur-Vaidman Bombs: The action of the beam splitter on a state $|\alpha\rangle + |\beta\rangle$ is of the form

$$\begin{pmatrix} s & u \\ t & v \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{1.12}$$

For a balanced beam splitter we have $\|s\|^2 = \|t\|^2 = \|u\|^2 = \|v\|^2$ and we can choose them, non uniquely, as

$$\begin{pmatrix} s & u \\ t & v \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \tag{1.13}$$

The action of the interferometer is of the form

$$BS_2 BS_1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ -\alpha \end{pmatrix} \tag{1.14}$$

When blocking the lower beam at BS_2 and act on $(0\ \ 1)$ we get

$$\begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix} \tag{1.15}$$

So, the resulting probabilities of hitting detector 0, detector 1 and the block is, respectively, 1/4, 1/4 and 1/2. By chaining these interferometers in a clever way one can reduce the probability of hitting the block such that it would be safe to test if a bomb activated by the detection of a photon works or not, without triggering the bomb with a high probability.

End of Lecture 2

1.5 The photoelectric effect

1. When radiating a polished metal, if the frequency of light exceeds a certain threshold frequency $\nu > \nu_0$ (which depends on the metal and the crystalline structure of it) a current flows through it, i.e. electrons start moving.

2. Increasing the intensity of the light, i.e. the number of photons per second per m^2 (but not the frequency of individual photons) increases the amount of ejected electrons but not their individual energy. Magnitude of the current is proportional to the light intensity. The energy of electrons is independent on the light intensity. Furthermore the energy of the electrons increases with the frequency of the light.

Einstein: Light is composed of individual packets of energy (quanta - photons) with energy $E = h\nu$. The work function W is the necessary energy to eject an electron. The energy of an electron should be

$$E_e = 1/2 m_e v^2 = E_\gamma - W = h\nu - W. \tag{1.16}$$

To remember, for easier calculations, $\hbar c \approx 200 MeV \cdot fm$.

Dimensional analysis of h:

$$[h] = \frac{[E]}{[\nu]} = \frac{ML^2/T^2}{1/T} = LM\frac{L}{T}, \tag{1.17}$$

which are units of angular momentum, distance times momentum.

1.6 Compton Scattering

The **Compton wavelength** of a particle: $h/(mc)$ (not to confuse with de Broglie wavelength). Corresponds to the wave length of a photon whose energy matches the rest energy of the particle. The relativistic mass-energy relation is given by

$$E^2 - p^2c^2 = m^2c^4. \tag{1.18}$$

The photon, with zero mass, has momentum given by

$$E_\gamma = p_\gamma c \implies p_\gamma = h\nu_\gamma/c = h/\lambda_\gamma. \tag{1.19}$$

Photons scattering on electrons that are virtually free (photon energy >> electron binding energy). From a photon electron collision we get

$$\lambda_f - \lambda_i = \frac{h}{m_e c}(1 - \cos\theta), \tag{1.20}$$

where $h/m_e c$ is the Compton wavelength of the electron.

1.7 de Broglie wave/particle duality

A particle with momentum p is associated to a plane wave of wavelength $\lambda = h/p$, called the de Broglie wavelength. This was verified experimentally via the famous double-slit experiment by Davisson and Germer. So particles interfere with each other by this wave-like behavior. See for example the following videos video 1 and video 2.

Observations which lead to the necessity of a quantum theory.

End of Lecture 3

1.8 Deriving Matter Waves (Wave Function)

Free particles have associated to them a plane wave of wavelength $\lambda = h/p$ (de Broglie). This matter wave is represented by the wave function $\Psi(\vec{x}, t) \in \mathbb{C}$ which is governed by Schrödinger's equation.

Let us consider what happens to the wavelength under a Galilean boost. Take an inertial frame S and another inertial frame S' with speed v along the x direction with coinciding time when they intersect. We have then

$$\begin{cases} x' = x - vt \\ t' = t. \end{cases} \tag{1.21}$$

Consider a particle moving with velocity $\bar{v}$ along the x direction. We have

$$\frac{dx'}{dt'} = \bar{v}' = \frac{dx}{dt}\frac{dt}{dt'} - v\frac{dt}{dt'} = \bar{v} - v. \tag{1.22}$$

Then

$$\lambda' = \frac{h}{p'} = \frac{h}{m(\bar{v} - v)} = \frac{h}{p - mv} \neq \frac{h}{p} = \lambda. \tag{1.23}$$

So, two inertial observers won't agree on the wavelength of the matter wave, it is not invariant to Galilean boosts. This in contrast to what happens to ordinary waves propagating in a medium.

Ordinary Waves (non-relativistic): Consider the phase of an ordinary wave in a medium

$$\phi = kx - \omega t = \frac{2\pi}{\lambda}x - \frac{2\pi\nu}{\lambda}t, \tag{1.24}$$

where k is the wave number and $\nu = \omega/k$ is the wave velocity. Two inertial observers must agree with the observed phase $\phi = \phi'$, when referring to the same point at the same time (imagine a water wave with a fixed observer and one moving towards the source). Thus

$$\phi' = \frac{2\pi}{\lambda}(x' + vt' - \nu t') = \frac{2\pi}{\lambda}x' - \frac{2\pi}{\lambda}\nu(1 - v/\nu)t'. \tag{1.25}$$

Reading the wave number as the factor on x' and the wave velocity as the t' factor and comparing to the wave in the frame S we conclude that

$$\begin{cases} k' = k \implies \lambda' = \lambda, \\ \omega' = (1 - v/\nu)\omega. \end{cases} \tag{1.26}$$

Remark 1.2. *It is not quite clear to me why we can keep λ and not write λ', isn't this assuming what we want to prove somewhat? Same hold for the wave velocity ν'.*

This matter wave does not behave like a regular wave, we conclude that ψ, this matter wave, can not be directly measured since two inertial observers won't agree on its value. The phase of matter waves are not Galilean invariant.

What is the frequency of this matter waves? By analogy with the energy of a photon we have $E = \hbar\omega$ and therefore we write $\omega = E/\hbar$, with the frequency being given by the energy. This is a postulate of quantum mechanics by de Broglie.

Wave velocities: The phase velocity is obtained simply by considering

$$kx - \omega t = C, \tag{1.27}$$

which, taking the time derivative, leads to

$$v_{phase} = \frac{dx}{dt} = \frac{\omega}{k} = \frac{E}{p} = \frac{1/2mv^2}{mv} = \frac{v}{2}, \tag{1.28}$$

which is suspicious. The group velocity turns out to be the quantity of interest (this means that a matter wave is actually a superposition of waves?)

$$v_{group} = \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{dE}{dp} = \frac{d}{dp}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = v. \tag{1.29}$$

Group velocity: The velocity of a wave packet constructed by a superposition of waves. Given $\omega(k)$ a superposition wave Ψ is of the form

$$\Psi(x,t) = \int \phi(k) e^{i(kx - \omega(k)t)} dk, \tag{1.30}$$

with $\varphi(k) = (kx - \omega(k)t)$ the phase of the wave. We assume that $\phi(k)$ is extremely localized and peaks around a certain value k_0.

Principle of stationary wave: Basically, if a function varies little and is multiplied by a *sin* or *cos* function of high frequency then the integral contribution of this portion is very small. Essentially, the contribution will come from places where the phase is stationary. Only when the phase stops varying fast with respect to k.

In our case, we need the phase to be stationary around $k = k_0$. This corresponds to

$$\left.\frac{d\varphi}{dk}\right|_{k_0} = 0 = x - \frac{d\omega}{dk}t \implies \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{x}{t}. \tag{1.31}$$

For a more rigorous argument we actually need to compute the integral. We have

$$\Psi(x,0) = \int \phi(k) e^{ikx} dk. \tag{1.32}$$

Expanding $\omega(k)$ around k_0 we get

$$\omega(k)|_{k_0} = \omega(k_0) + \frac{d\omega}{dk}(k_0)(k-k_0) + \mathcal{O}((k-k_0)^2). \tag{1.33}$$

So, the integral becomes

$$\Psi(x,t) \approx \int \phi(k) e^{i(kx-(\omega(k_0)+\frac{d\omega}{dk}(k_0)(k-k_0)))t)} dk = e^{-i\omega(k_0)t} e^{ik_0 \frac{d\omega}{dk}(k_0)t} \int \phi(k) e^{ik(x-\frac{d\omega}{dk}(k_0)t)}. \tag{1.34}$$

Then, by comparison with $\Psi(x,0)$ we have

$$|\Psi(x,t)| \approx \left| \Psi\left(x - \frac{d\omega}{dk}(k_0)t, 0\right) \right|, \tag{1.35}$$

so we conclude that the group velocity is $\frac{d\omega}{dk}(k_0)$.

Remark 1.3. *This is only exact when $\omega(k)$ is linear in k.*

Matter Wave: The matter wave (or wave function) is of the form (via a neat argument see video 20)

$$\Psi(x,t) = e^{ikx - i\omega t}, \tag{1.36}$$

for a particle with $E = \hbar\omega$, $p = \hbar k$. And, for a non-relativistic particle, $E = p^2/2m$.

End of Lecture 4

The main question now is: What is the equation that governs the wave function of a particle?

1.9 Schrödinger's Equation

We start with a matter wave solution $\psi(x,t) = e^{i(kx-\omega t)}$ and observe that

$$\underbrace{\frac{\hbar}{i}\frac{\partial}{\partial x}}_{\hat{p}} \psi = \hbar k \psi = p\psi. \tag{1.37}$$

Similarly

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{\hat{E}} \psi = \hbar\omega\psi = E\psi. \tag{1.38}$$

We call $\hat{p}$ and $\hat{E}$ the momentum and energy operators and, when the above equations are satisfied, we say that ψ is an eigenstate of these operators with eigenvalues p and E. Recalling that, non-relativistically, $E = p^2/2m$, we can further write

$$\frac{1}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\right) = \frac{p^2}{2m}\psi, \tag{1.39}$$

or

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = \frac{p^2}{2m}\psi = E\psi. \tag{1.40}$$

Relating the two operator for energy we obtain

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{1.41}$$

This last PDE is the equation that ends up governing the matter wave and is known as the **free Schrödinger's equation**. By linearity, the general solution to this equation is of the form

$$\psi(x,t) = \int_{-\infty}^{\infty} \phi(k)e^{i(kx-\omega(k)t)}dk, \tag{1.42}$$

with group velocity $v_g = (d\omega/dk)(k_0)$, assuming $\phi(k)$ is peaked at k_0. Note that ψ can not be real for the equation to make sense.

Suppose now that the particle moves in a potential $V(x,t)$ then $E = K + V$ and

$$i\hbar\frac{\partial}{\partial t}\psi = E\psi = \left(\frac{p^2}{2m} + V\right)\psi. \tag{1.43}$$

But, from (1.40), we can write

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{1.44}$$

This is the full Schrödinger's equation and one usually calls

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(x,t) = \hat{H}, \tag{1.45}$$

the Hamiltonian operator.

Remark 1.4. *The sum of an operator and the potential function seems a bit odd, they are different objects so their sum as no real meaning a priori. One defines $V(x,t)$ as the operator that multiplies a function by $V(x,t)$. One can then define a space of these operators where the sum makes sense by their application on the space of smooth functions.*

Defining the position operator $\hat{x}\phi = x\phi$ we can look at the commutator with the momentum, by a simple computation we obtain

$$[\hat{x},\hat{p}]\phi = i\hbar\phi. \tag{1.46}$$

We have then

$$[\hat{x},\hat{p}] = i\hbar. \tag{1.47}$$

The relation between the Schrödinger picture VS the Heisenberg picture (matrix picture) is the following

- Operators $\longleftrightarrow$ Matrices.
- Wave functions $\longleftrightarrow$ Vectors.
- Eigenstates or Eigenfunctions $\longleftrightarrow$ Eigenvectors.

Schrödinger's Equation in 3D

In 3D, by de Broglie, one has $\vec{p} = \hbar\vec{k}$ and the matter wave is of the form

$$\psi(\vec{x},t) = e^{i(\vec{k}\cdot\vec{x}-\omega t)}, \tag{1.48}$$

where

$$\hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}. \tag{1.49}$$

Since

$$\hat{\vec{p}}\hat{\vec{p}} = -\hbar^2\nabla^2 = -\hbar^2\Delta, \tag{1.50}$$

the Schrödinger equation becomes

$$\left(-\frac{\hbar^2}{2m}\Delta + V(\vec{x},t)\right)\psi(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t). \tag{1.51}$$

The commutator relations become

$$[\hat{x_i}, \hat{p_j}] = i\hbar\delta_{ij}. \tag{1.52}$$

1.10 Interpreting the Wave Function

The value of $\psi(x,t)$ itself has no physical interpretation, we interpret instead $|\psi(x,t)|^2$ as the probability of finding the particle at position x and at time t. Since a continuous probability function has zero probability pointwise we interpret this in the following way

$$dP(\vec{x},t) = |\psi(\vec{x},t)|^2 d^3x, \tag{1.53}$$

the volume of a small cube of side dx. Naturally, like every probability distribution, we should have

$$\int_{\mathbb{R}^3} |\psi(\vec{x},t)|^2 dV = 1, \tag{1.54}$$

which means physically that the particle should be somewhere. Since Schrödinger's equation tells us how the wave function evolves in time, in order for this to be consistent this above relation should be satisfied for all times, i.e. the Schrödinger's equation must keep the wave function normalized.

End of Lecture 5

1.11 Normalizable Wave Functions

So, in 1 dimension, we require that

$$\int_{\mathbb{R}} \Psi(x,t)\Psi^*(x,t)dx = 1, \tag{1.55}$$

at all times. It clearly must hold that (modulo "strange wavefunctions")

$$\lim_{x\to\pm\infty} \Psi(x,t) = 0. \tag{1.56}$$

We also ask that

$$\lim_{x\to\pm\infty} \frac{\partial\Psi}{\partial x} \text{ is bounded.} \tag{1.57}$$

Since complex numbers are not ordered this actually means that

$$\lim_{x\to\pm\infty} \left|\frac{\partial\Psi}{\partial x}\right| \leq M, \tag{1.58}$$

for some $M \in \mathbb{R}$. If

$$\int_{\mathbb{R}} \Psi(x,t)\Psi^*(x,t)dx = N, \;\; N \in \mathbb{R}, \tag{1.59}$$

then Ψ is normalizable by taking $\Psi' = \Psi/\sqrt{N}$.

We now turn to the starting question that is: does the evolution of the wave function given by Schrödinger's equation keep this normalization?

Define the probability density

$$\rho(x,t) := \Psi^*(x,t)\Psi(x,t), \tag{1.60}$$

and

$$\mathcal{N}(t) = \int_{\mathbb{R}} \rho(x,t)dx, \tag{1.61}$$

where $\mathcal{N}(t_0) = 1$. The question can now be formulated as: will the Schrödinger equation guarantee that $d\mathbf{N}/dt = 0$? We have

$$\begin{aligned} \frac{d\mathcal{N}(t)}{dt} &= \int_{\mathbb{R}} \frac{\partial \rho(x,t)}{\partial t} dx = \int_{\mathbb{R}} \left(\frac{\partial \Psi^*(x,t)}{\partial t}\Psi(x,t) + \Psi^*(x,t)\frac{\Psi(x,t)}{\partial t} \right) dx \\ &= \int_{\mathbb{R}} \frac{i}{\hbar} \left[(\hat{H}\Psi)^*\Psi - \Psi^*(\hat{H}\Psi) \right] dx, \end{aligned} \tag{1.62}$$

using from Schrödinger's equation that

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\Psi, \tag{1.63}$$

and that the complex conjugate of Schrödinger's equation is

$$\begin{aligned} -i\hbar \left(\frac{\partial \Psi}{\partial t} \right)^* &= (\hat{H}\Psi)^* \\ \Leftrightarrow \quad \frac{\partial \Psi^*}{\partial t} &= \frac{i}{\hbar}(\hat{H}\Psi)^*. \end{aligned} \tag{1.64}$$

Equation (1.62) being equal to zero is equivalent to

$$\int_{\mathbb{R}} (\hat{H}\Psi)^*\Psi dx = \int_{\mathbb{R}} \Psi^*(\hat{H}\Psi)dx. \tag{1.65}$$

This holds if $\hat{H}$ is an Hermitian operator, i.e. if

$$\int_{\mathbb{R}} (\hat{H}\Psi)^*\Phi dx = \int_{\mathbb{R}} \Psi^*(\hat{H}\Phi)dx, \tag{1.66}$$

for any two wave functions Ψ and Φ. In general, one defines

Definition 1.2. ***(Hermitian Conjugate)***

Given an operator $\hat{\mathcal{O}}$ we define its Hermitian conjugate $\hat{\mathcal{O}}^\dagger$ by

$$\int_{\mathbb{R}} \Psi^*\hat{\mathcal{O}}\Phi dx = \int_{\mathbb{R}} (\hat{\mathcal{O}}^\dagger\Psi)^*\Phi dx, \tag{1.67}$$

for any two vectors Ψ and Φ. We say that an operator $\hat{\mathcal{O}}$ is Hermitian if

$$\hat{\mathcal{O}}^\dagger = \hat{\mathcal{O}}. \tag{1.68}$$

Going back to the calculation using the fact that we know $\hat{H}$ and $V(x,t) \in \mathbb{R}$ we get

$$\begin{aligned}\frac{\partial \rho(x,t)}{\partial t} &= \frac{i}{\hbar}\left[(\hat{H}\Psi)^*\Psi - \Psi^*(\hat{H}\Psi)\right] \\ &= \frac{i}{\hbar}\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi\right)^*\Psi - \Psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi\right)\right] \\ &= \frac{i}{\hbar}\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + V\Psi^*\right)\Psi + \Psi^*\left(\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - V\Psi\right)\right] \\ &= \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right).\end{aligned} \tag{1.69}$$

We get then, by the Fundamental Theorem of Calculus, that

$$\begin{aligned}&\frac{i\hbar}{2m}\int_{\mathbb{R}}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)dx = \frac{i\hbar}{2m}\int_{\mathbb{R}}\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)dx \\ =&\frac{i\hbar}{2m}\left[\Psi^*\Big|_{+\infty}\frac{\partial\Psi}{\partial x}\Big|_{+\infty} - \frac{\partial\Psi^*}{\partial x}\Big|_{+\infty}\Psi\Big|_{+\infty} - \left(\Psi^*\Big|_{-\infty}\frac{\partial\Psi}{\partial x}\Big|_{-\infty} - \frac{\partial\Psi^*}{\partial x}\Big|_{-\infty}\Psi\Big|_{-\infty}\right)\right] = 0,\end{aligned} \tag{1.70}$$

and this is zero by assumptions (1.56) and (1.57).

Remark 1.5. *This evaluations at infinity are, rigorously, all limits.*

Notice that

$$\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi, \tag{1.71}$$

is of the form $z - z^* = 2iIm(z)$, and

$$\frac{\partial\rho}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{\hbar}{m}Im\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right], \tag{1.72}$$

we call

$$J(x,t) = \frac{\hbar}{m}Im\left(\Psi^*\frac{\partial\Psi}{\partial x}\right), \tag{1.73}$$

the current density such that

$$\frac{\partial\rho}{\partial t} = -\frac{\partial J}{\partial x}, \tag{1.74}$$

or equivalently

$$\frac{\partial\rho}{\partial t} + \frac{\partial J}{\partial x} = 0. \tag{1.75}$$

This is the equation for current conservation. By dimensional analysis one can check that $[J] = T^{-1}$, a probability current, i.e. probability per unit time. In 3 dimensions one obtains

$$\vec{J} = \frac{\hbar}{m}Im\left(\Psi^*\nabla\Psi\right), \tag{1.76}$$

and

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = 0. \tag{1.77}$$

This equations essentially tells us that when the probability density changes in a region its due to a probability current through the boundary of this region. This can be seen clearly by the Divergence Theorem, given a charge Q contained in a bounded volume V we have

$$Q = \int_V \rho(\vec{x},t)dV. \tag{1.78}$$

Then

$$\frac{dQ}{dt} = \int_V \frac{\partial \rho}{\partial t}(\vec{x}, t) dV = -\int_V \nabla \cdot \vec{J} dV = -\int_{\partial V} \vec{J} \cdot \hat{n} dS, \tag{1.79}$$

where $\hat{n}$ is the normal vector to the boundary. By dimensional analysis one can check that $[J] = L^{-2}T^{-1}$, probability per unit area and unit time. Since

$$\frac{d\mathcal{N}(t)}{dt} = \int_{\mathbb{R}} \frac{\partial \rho}{\partial t} dx = -\int_{\mathbb{R}} \frac{\partial J}{\partial x} dx = J(x = -\infty, t) - J(x = +\infty, t) = 0. \tag{1.80}$$

Remark 1.6. *Again, these are limits.*

To finalize, interpreting the current conservation equation in 1D in an interval $I = [a, b]$ we have essentially

$$\left.\frac{dP}{dt}\right|_I = \int_a^b \frac{\partial \rho(x,t)}{\partial t} dx = -\int_a^b \frac{\partial J}{\partial x}(x,t) dx = J(a,t) - J(b,t). \tag{1.81}$$

Which means that the variation in probability of finding the particle in the interval changes by the probability current entering through $x = a$ and leaving through $x = b$.

The most important points here are that indeed the evolution of a state by Schrödinger's equation maintains its normalization if $\hat{H}$ is an Hermitian operator and this leads to the existence of a probability current $\vec{J}$ and probability conservation equation.

End of Lecture 6

1.12 Wave Packets and Fourier Representation

Review

Nice sequence of videos by Grant Sanderson (3blue1brown) to better understand the following lectures: Euler's Formula $\longrightarrow$ Fourier Transform $\longrightarrow$ Uncertainty Principle.

The main defining property of e is the fact that

$$\frac{d}{dt}\left(a^t\right) = \ln(a) a^t, \tag{1.82}$$

such that

$$\frac{d}{dt}\left(e^t\right) = e^t, \tag{1.83}$$

has a proportionality constant of 1. Introducing complex numbers, we have

$$\frac{d}{dt}\left(e^{it}\right) = ie^{it}, \tag{1.84}$$

which means that if e^{it} corresponds to a position in the complex plane of a particle, then its velocity is a vector at 90° of the same length. The integral curve of such a vector field leads to a circle. So, essentially

$$f(t) = e^{i\omega t}, \tag{1.85}$$

traces the position around a circle covered at a certain angular velocity ω. If $\omega = \pi/2$, after 1 unit of time, the particle is at $(0, i)$ while if $\omega = 2\pi$ the particle stands at $(1, 0)$ after 1 unit of time. Summarizing, ω dictates the arc-length traveled by the particle per unit time.

Suppose we have two pure sound waves of a certain frequency whose amplitude is given by

$$f_i(t) = A_i cos(\omega_i t), \;\; i = 1, 2, \tag{1.86}$$

and we take their sum

$$g(t) = A_1 cos(\omega_1 t) + A_2 cos(\omega_2 t). \tag{1.87}$$

The question is, can we, from observing $g(t)$, recover the individual frequencies composing it?
To achieve this, we consider a vector, with length equal to the amplitude of $f_i(t)$ for example, rotating in the complex plane as a function of time. This wraps the signal around the circle and we can choose how many seconds corresponds to a rotation around this circle, which leads to a different frequency, independent from the signal's frequency given by $\omega' = 2\pi/t'$, where t' is the time it takes to go around the circle.
When the winding frequency ω' is close to ω_i something special happens, all the high points occur on the right and all the low points occur on the left (assuming the peak occurs at $t = 0$).
The next step is to consider the geometric centroid of this winded up signal. The key observation here is that this centroid stays close to the origin except when $\omega' \approx \omega_i$. Crucially, if we take the distance of this centroid as a function of time of two different signal and add them up, this is equivalent to summing the signals and then performing this winding plus centroid computation.
So, back to the start, a way to capture this winding behavior is by taking $e^{i\omega t}$, which rotates around the circle of radius 1 at 1 cycle/s, i.e. one full rotation around the circle per second. The convention is to consider rotations in the clockwise direction and so we take instead $e^{-i\omega t}$.
Taking our original signal, amplitude per time $g(t)$, then

$$g(t)e^{-i\omega t}, \tag{1.88}$$

corresponds to a winding of the signal around the circle with an angular frequency given by ω. Finally the centroid position in the complex plane is given by

$$\frac{1}{T}\int_0^T g(t)e^{-i\omega t}dt, \tag{1.89}$$

for some $T \in \mathbb{R}$. The actual Fourier Transform is defined as

$$\hat{g}(\nu) = \int_{\mathbb{R}} g(t)e^{-i2\pi\nu t}dt, \tag{1.90}$$

or

$$\hat{g}(\omega) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} g(t)e^{-i\omega t}dt, \tag{1.91}$$

with corresponding inverse transforms.

Remark 1.7. *Just a quick note regarding Heisenberg's uncertainty principle. It isn't so much it being a weird feature of quantum mechanics, it's an imposed feature by the wave description of matter as matter waves. For a sound wavew, the intuitive trade-off between a localized pulse in time and uncertainty regarding its frequency translates to a localized pulse in space translating to uncertainty in momentum, i.e. $p = \hbar\nu$, the frequency.*

Consider, by the Fourier transform,

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi(k) e^{ikx} dk, \tag{1.92}$$

and, by the inverse transform

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Psi(x,0) e^{-ikx} dx, \tag{1.93}$$

with $\Phi(k) \in \mathbb{R}$ peaked around k_0 with uncertainty Δk and $\|\Psi(x,0)\|$ peaking around x_0 with uncertainty Δx. Suppose we want to check that $\Psi(x,0)$ is a real number.

Remark 1.8. *This does not contradict the fact that $\Psi(x,t) \in \mathbb{C}$, as we have seen before, since the time evolution introduces a complex phase.*

We check if

$$\Psi(x,0) = \Psi^*(x,0), \tag{1.94}$$

is satisfied. We have

$$\Psi^*(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi^*(k) e^{-ikx} dk. \tag{1.95}$$

Changing variable to $k' = -k$, we obtain

$$\Psi^*(x,0) = -\frac{1}{\sqrt{2\pi}} \int_{+\infty}^{-\infty} \Phi^*(-k') e^{ik'x} dk' = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi^*(-k) e^{ikx} dk, \tag{1.96}$$

using the properties for definite integrals and relabeling k' to k. If we look at $\Psi(x,0) - \Psi^*(x,0)$ we have

$$\Psi(x,0) - \Psi^*(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\Phi(k) - \Phi^*(-k)\right) e^{ikx} dk. \tag{1.97}$$

If $\Psi(x,0)$ is to be a real number the above expression must vanish for all values of k. To argue that this implies

$$\Phi(k) - \Phi^*(-k) = 0, \tag{1.98}$$

for all k we need to be careful. The equation

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\Phi(k) - \Phi^*(-k)\right) e^{ikx} dk = 0, \tag{1.99}$$

implies that the Fourier transform of the function $\Phi(k) - \Phi^*(-k)$ vanishes identically. Thus, by the inverse Fourier transform we conclude that $\Phi(k) - \Phi^*(-k) = 0$, i.e.

$$\Phi(k) = \Phi^*(-k). \tag{1.100}$$

This however contradicts our initial choice of $\phi \in \mathbb{R}$ being peaked at $k = k_0$ and close to zero at $-k$ and thus $(\phi(-k_0))^* \approx 0$. We now consider the Fourier transform integral around k_0 taking $k = k_0 + \tilde{k}$, valid since we assume $\phi(k)$ peaked at k_0, and therefore

$$\begin{aligned} \Psi(x,0) &= \frac{1}{\sqrt{2\pi}} e^{ik_0 x} \int_{\mathbb{R}} \Phi(k_0 + \tilde{k}) e^{i\tilde{k}x} d\tilde{k} \\ &= \frac{1}{\sqrt{2\pi}} e^{ik_0 x} \int_{-\frac{\Delta k}{2}}^{\frac{\Delta k}{2}} \Phi(k_0 + \tilde{k}) e^{i\tilde{k}x} d\tilde{k}. \end{aligned} \tag{1.101}$$

The total variation of the phase factor, $\tilde{k}x$, is from $[-x\Delta k/2, x\Delta k/2]$ or of length $x\Delta k$. Thus, if $x\Delta k \lesssim 1$, we are in the condition of a stationary phase and we get a contribution to the integral, otherwise, the phase changes too quickly around k_0 and the contribution to the integral vanishes (see the stationary phase argument above). This happens if $x\Delta k \gg 1$. To conclude, $\Psi(x,0)$ is sizeable in the interval $(-x_0, x_0)$ if $x\Delta k \approx 1$, $\Delta x = 2x_0$ and $\Delta x \Delta k \approx 1$ (is of the order of). This is just a consequence of wave packets and Fourier's Transform (as mentioned before). If we recall, from quantum mechanics, that $\Delta p = \hbar \Delta k$ we get

$$\Delta p \Delta k \approx \hbar. \tag{1.102}$$

The accurate result, using the correct definitions, leads to

$$\Delta p \Delta k \geq \frac{\hbar}{2}. \tag{1.103}$$

1.13 Time Evolution of a Free Particle

Suppose we know $\Psi(x,0)$.

- Step 1: First, by Fourier's Transform, we calculate

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Psi(x,0) e^{-ikx} dx. \tag{1.104}$$

- Step 2: Rewrite, again by Fourier's Transform,

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi(k) e^{ikx} dk. \tag{1.105}$$

  The achievement in doing this is that we get to obtain $\Psi(x,0)$, an arbitrary function, as a superposition of plane waves.

  Remark 1.9. *The actual point is the following: for a free particle, writing $\Psi(x,t)$ as a superposition of plane waves and substituting back into Schrödinger's equation simply gives an ODE for $\Phi(k,t)$, i.e.*

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t). \tag{1.106}$$

  By Fourier Transform we have

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k,t)\, e^{ikx}\, dk. \tag{1.107}$$

  The time derivative is given by

$$\frac{\partial \Psi(x,t)}{\partial t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\partial \phi(k,t)}{\partial t}\, e^{ikx}\, dk, \tag{1.108}$$

  while the second order spatial derivative is given by

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k,t)\, \frac{\partial^2}{\partial x^2} e^{ikx}\, dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (-k^2)\, \phi(k,t)\, e^{ikx}\, dk. \tag{1.109}$$

  Thus, substituting back into (1.106) we get

$$i\hbar \frac{1}{\sqrt{2\pi}} \int \frac{\partial \phi(k,t)}{\partial t}\, e^{ikx}\, dk = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{2\pi}} \int (-k^2)\, \phi(k,t)\, e^{ikx}\, dk. \tag{1.110}$$

Which leads to

$$i\hbar \int \frac{\partial \phi(k,t)}{\partial t}\, e^{ikx}\, dk = \frac{\hbar^2}{2m} \int k^2\, \phi(k,t)\, e^{ikx}\, dk. \tag{1.111}$$

Since the exponential functions $\{e^{ikx}\}$ *form a complete orthogonal basis, the integrands must match at each* k*, therefore*

$$i\hbar\, \frac{\partial \phi(k,t)}{\partial t} = \frac{\hbar^2 k^2}{2m}\, \phi(k,t) = \frac{p^2}{2m}\, \phi(k,t). \tag{1.112}$$

This is the Schrödinger equation in momentum space and the solution is just

$$\phi(k,t) = \phi(k,0)\, e^{-i\frac{\hbar k^2}{2m}t}. \tag{1.113}$$

- Step 3: From step 2, at a later time t we just evaluate

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi(k) e^{i(kx-\omega(k)t)} dk, \tag{1.114}$$

where $\hbar\omega(k) = E = p^2/(2m) = \hbar^2 k^2/(2m)$. Furthermore, $\Psi(x,t)$ verifies the Schrödinger's equation with initial condition $\Psi(x,0)$ at $t = 0$.

- Step 4: Compute the above integral in k.

End of Lecture 7

1.14 Momentum Space

The first observation is that, through Fourier's Theorem, $\Phi(k)$ has the same information as $\Psi(x)$. We have

$$\begin{aligned} \Psi(x) &= \frac{1}{2\pi} \int_{\mathbb{R}} \left(\int_{\mathbb{R}} \Psi(x') e^{-ikx'} dx' \right) e^{ikx} dk \\ &= \int_{\mathbb{R}} \Psi(x') \left(\frac{1}{2\pi} \int_{\mathbb{R}} e^{ik(x-x')} dk \right) dx', \end{aligned} \tag{1.115}$$

by Fubini's Theorem, since we assume that our functions are absolutely integrable, i.e. have finite L^1 norm.

Remark 1.10. *There are some interesting subtleties here in regards to function spaces because wave functions live in Hilbert spaces,* $L^2(\mathbb{R}, \mathbb{C})$*, which is not contained in* L^1*. Typically in physics one considers the Schwarz space* $\mathcal{S}$*, i.e. the space of smooth and rapidly decaying functions which is dense in* L^2*.*

We define the "function" (rigorously a distribution)

$$\delta(x' - x) := \frac{1}{2\pi} \int_{\mathbb{R}} e^{ik(x'-x)} dk, \tag{1.116}$$

by changing variable $k' = -k$ and relabeling it as k again. This essentially extracts from the full integral in x', the value of Ψ at x.

We now want to check the normalization condition for $\Phi(k)$. We have

$$\begin{aligned} \int_{\mathbb{R}} |\Psi(x)|^2 dx &= \int_{\mathbb{R}} \Psi^*(x)\Psi(x) dx \\ &= \int_{\mathbb{R}} \left[\left(\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi^*(k) e^{-ikx} dk \right) \left(\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi(k') e^{ik'x} dk' \right) \right] dx. \end{aligned} \tag{1.117}$$

Let us define

$$f(x) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi^*(k) e^{-ikx} dk, \tag{1.118}$$

$$g(x) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi(k') e^{ik'x} dk', \tag{1.119}$$

and

$$\tilde{f}(k) := \frac{1}{\sqrt{2\pi}} \Phi^*(k) e^{-ikx}. \tag{1.120}$$

$$\tilde{g}(k') := \frac{1}{\sqrt{2\pi}} \Phi(k') e^{ik'x}. \tag{1.121}$$

By Fubini's Theorem, the above integral is then

$$\begin{aligned}
\int_{\mathbb{R}} \left[\int_{\mathbb{R}} \left(g(x) \tilde{f}(k) \right) dk \right] dx &= \int_{\mathbb{R}} \left[\int_{\mathbb{R}} \left(g(x) \tilde{f}(k) \right) dx \right] dk \\
&= \int_{\mathbb{R}} \left[\int_{\mathbb{R}} \left(\left(\int_{\mathbb{R}} \tilde{g}(k') dk' \right) \tilde{f}(k) \right) dx \right] dk \\
&= \int_{\mathbb{R}} \left[\int_{\mathbb{R}} \left(\left(\int_{\mathbb{R}} \tilde{g}(k') \tilde{f}(k) \right) dx \right) dk' \right] dk \\
&= \int_{\mathbb{R}} \left[\Phi^*(k) \int_{\mathbb{R}} \left[\Phi(k') \underbrace{\left(\int_{\mathbb{R}} \left(\frac{1}{2\pi} e^{-ix(k'-k)} \right) dx \right)}_{\delta(k'-k)} \right] dk' \right] dk \\
&= \int_{\mathbb{R}} \left[\Phi^*(k) \Phi(k) \right] dk = \int_{\mathbb{R}} |\Phi(k)|^2 dk.
\end{aligned} \tag{1.122}$$

This is called Parseval's Theorem. Thus, if

$$\int_{\mathbb{R}} |\Psi(x)|^2 dx = 1, \tag{1.123}$$

we have

$$\int_{\mathbb{R}} |\Phi(k)|^2 dk = 1, \tag{1.124}$$

and this holds for all time t. So, we can interpret this again as a probability distribution but now over momentum space. Rewriting Fourier's Theorem as a function of $p = \hbar k$, we have

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Phi(k) e^{ipx\hbar} dk, \tag{1.125}$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Psi(x) e^{-ipx\hbar} dx. \tag{1.126}$$

This change in normalization maintains Parseval's Theorem, i.e.

$$\int_{\mathbb{R}} |\Psi(x)|^2 dx = \int_{\mathbb{R}} |\Phi(p)|^2 dp = 1. \tag{1.127}$$

Thus, $|\Phi(p)|^2 dp$ is the probability of finding the particle with momentum $[p, p + dp]$. In 3-dimensional space the equivalent expressions of the above are given by

$$\Psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \Phi(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} d^3p. \tag{1.128}$$

$$\Psi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \Psi(\vec{x}) e^{-i\vec{p}\cdot\vec{x}/\hbar} d^3x. \tag{1.129}$$

$$\delta^3(\vec{x'} - \vec{x}) := \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{i\vec{k}\cdot(\vec{x'}-\vec{x})} dk, \tag{1.130}$$

and

$$\int_{\mathbb{R}^3} |\Psi(\vec{x})|^2 d^3x = \int_{\mathbb{R}^3} |\Phi(\vec{p})|^2 d^3p = 1. \tag{1.131}$$

1.15 Expectation Values of Operators

Recall the definition of the expectation value for a discrete random variable Q with sample space in the set $\{q_1, q_2, ..., q_n\}$ with respective probabilities $\{p_1, p-2, ..., p_n\}$.

$$\mathbb{E}(Q) = \langle Q \rangle := \sum_{i=1}^{n} q_i p_i. \tag{1.132}$$

For a continuous distribution supported in $\mathbb{R}$ we have

$$\mathbb{E}(Q) = \langle Q \rangle := \int_{\mathbb{R}} qp(Q = q)dq. \tag{1.133}$$

Recalling that

$$\Psi^*(x,t)\Psi(x,t)dx = |\Psi(x,t)|^2, \tag{1.134}$$

corresponds to the probability of finding the particle in the interval $[x, x + dx]$ we have

$$\langle \hat{x} \rangle(t) := \int_{\mathbb{R}} x|\Psi(x,t)|^2 dx. \tag{1.135}$$

Similarly, as said above,

$$\Phi^*(p,t)\Phi(p,t)dp = |\Phi(p,t)|^2, \tag{1.136}$$

corresponds to the probability of the particle having momentum p in the interval $[p, p + dp]$. Thus

$$\langle \hat{p} \rangle(t) := \int_{\mathbb{R}} p\Phi^*(p,t)\Phi(p,t)dp. \tag{1.137}$$

The question now is, how can we find $\langle \hat{p} \rangle(t)$ without changing first our wave function to momentum space? We have

$$\begin{aligned} \langle \hat{p} \rangle(t) &:= \int_{\mathbb{R}} \left[p \left(\frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Psi^*(x',t) e^{ipx'/\hbar} dx' \right) \left(\frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Psi(x,t) e^{-ipx/\hbar} dx \right) \right] dp \\ &= \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left[\Psi^*(x',t) \int_{\mathbb{R}} \left(\Psi(x,t) \int_{\mathbb{R}} p e^{ip(x'-x)/\hbar} dp \right) dx \right] dx'. \end{aligned} \tag{1.138}$$

We now look at the term

$$\int_{\mathbb{R}} p e^{ip(x'-x)/\hbar} dp, \tag{1.139}$$

which we can write as

$$i\hbar \int_{\mathbb{R}} \frac{\partial}{\partial x} \left(e^{ip(x'-x)/\hbar} \right) dp. \tag{1.140}$$

Therefore,

$$\begin{aligned} \langle \hat{p} \rangle(t) &= \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left[\Psi^*(x',t) \int_{\mathbb{R}} \left(\Psi(x,t) i\hbar \int_{\mathbb{R}} \frac{\partial}{\partial x} \left(e^{ip(x'-x)/\hbar} \right) dp \right) dx \right] dx' \\ &= \int_{\mathbb{R}} \left[\Psi^*(x',t) \int_{\mathbb{R}} \left(\Psi(x,t) i\hbar \frac{\partial}{\partial x} \underbrace{\left[\frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right]}_{\delta(x'-x)} \right) dx \right] dx'. \end{aligned} \tag{1.141}$$

We now do integration by parts to pass the derivative over the delta function to Ψ.

$$\begin{aligned} \int_{\mathbb{R}} \Psi^*(x',t) \Bigg(& \left[\frac{i}{2\pi} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right] \Psi(x,t) \Big|_{x=-\infty}^{x=\infty} \\ & - \int_{\mathbb{R}} \left(i\hbar \frac{\partial \Psi(x,t)}{\partial x} \right) \left[\frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right] dx \Bigg) dx' \end{aligned} \tag{1.142}$$

Since the delta function and the wave function decay extremely fast to zero, the boundary terms vanish and we obtain

$$\begin{aligned} & -\int_{\mathbb{R}} \Psi^*(x',t) \int_{\mathbb{R}} \left(i\hbar \frac{\partial \Psi(x,t)}{\partial x} \right) \left[\frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right] dx dx' \\ = & \frac{\hbar}{i} \int_{\mathbb{R}} \Psi^*(x',t) \int_{\mathbb{R}} \left(\frac{\partial \Psi(x,t)}{\partial x} \right) \delta(x-x') dx dx' \\ = & \int_{\mathbb{R}} \left[\frac{\hbar}{i} \frac{\partial \Psi}{\partial x}(x,t) \left(\int_{\mathbb{R}} (\Psi^*(x',t)\delta(x-x'))\, dx' \right) \right] dx \\ = & \int_{\mathbb{R}} \left[\frac{\hbar}{i} \frac{\partial \Psi}{\partial x}(x,t) \Psi^*(x,t) \right] dx. \end{aligned} \tag{1.143}$$

Notice that the delta function is even $\delta(x) = \delta(-x)$. So, we conclude that

$$\langle \hat{p} \rangle(t) = \int_{\mathbb{R}} \left[\Psi^*(x,t) \frac{\hbar}{i} \frac{\partial \Psi}{\partial x}(x,t) \right] dx, \tag{1.144}$$

where

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}. \tag{1.145}$$

In general we define

$$\langle \hat{Q} \rangle(t) = \int_{\mathbb{R}} \Psi^*(x,t) \hat{Q} \Psi(x,t) dx. \tag{1.146}$$

Remark 1.11. *This of course is not a logical conclusion from what happens with only the momentum operator. We take this as an axiom of quantum mechanics but is based on the general structure of how operators act on Hilbert spaces.*

Example: Take the kinetic energy operator

$$\hat{T} = \frac{\hat{p}^2}{2m}. \tag{1.147}$$

In momentum space, we simply have

$$\langle \hat{T} \rangle(t) = \int_{\mathbb{R}} \Phi^*(p,t) \frac{p^2}{2m} \Phi(p,t) dp. \tag{1.148}$$

In position space, we have

$$\begin{aligned} \langle \hat{T} \rangle(t) &= \int_{\mathbb{R}} \Psi^*(x,t) \frac{i}{\hbar} \frac{\partial}{\partial x} \left(\frac{i}{\hbar} \frac{\partial}{\partial x} \Psi(x,t) \right) dp \\ &= -\frac{\hbar^2}{2m} \int_{\mathbb{R}} \Psi^*(x,t) \frac{\partial^2 \Psi}{\partial x^2}(x,t) dx \\ &= \frac{\hbar^2}{2m} \int_{\mathbb{R}} \frac{\partial \Psi^*}{\partial x}(x,t) \frac{\partial \Psi}{\partial x}(x,t) dx = \frac{\hbar^2}{2m} \int_{\mathbb{R}} |\Psi(x,t)|^2 dx, \end{aligned} \tag{1.149}$$

using integration by parts.

Time dependence of expectation values: Assuming our operator Q has no time dependence we have

$$\begin{aligned} \frac{d}{dt} \langle \hat{Q} \rangle(t) &= \frac{d}{dt} \int_{\mathbb{R}} \Psi^*(x,t) \hat{Q} \Psi(x,t) dx. \\ &= \int_{\mathbb{R}} \left(\frac{\partial \Psi^*}{\partial t}(x,t) \hat{Q} \Psi(x,t) + \Psi^*(x,t) \hat{Q} \frac{\partial \Psi}{\partial t}(x,t) \right) dx. \end{aligned} \tag{1.150}$$

Using Schrödinger's equation we obtain

$$\begin{aligned} & \int_{\mathbb{R}} \left(\frac{\partial \Psi^*}{\partial t}(x,t) \hat{Q} \Psi(x,t) + \Psi^*(x,t) \hat{Q} \frac{\partial \Psi}{\partial t}(x,t) \right) dx \\ = & \int_{\mathbb{R}} \left(\frac{i}{\hbar} (\hat{H}\Psi)^* \hat{Q} \Psi - \Psi^* \frac{i}{\hbar} (\hat{Q} \hat{H} \Psi) \right) dx. \end{aligned} \tag{1.151}$$

Looking at

$$\begin{aligned} i\hbar\frac{d}{dt}\langle\hat{Q}\rangle(t) &= \int_{\mathbb{R}} \left(\Psi^*(\hat{Q}\hat{H}\Psi) - (\hat{H}\Psi)^*\hat{Q}\Psi\right) dx \\ &= \int_{\mathbb{R}} \left(\Psi^*(\hat{Q}\hat{H}\Psi) - \Psi^*\hat{H}\hat{Q}\Psi\right) dx \\ &= \int_{\mathbb{R}} \Psi^*(x,t)[\hat{Q},\hat{H}]\Psi(x,t)dx. \end{aligned} \tag{1.152}$$

So we found out that

$$i\hbar\frac{d}{dt}\langle\hat{Q}\rangle(t) = \langle[\hat{Q},\hat{H}]\rangle(t). \tag{1.153}$$

Remark 1.12. *In Schrödinger's picture of quantum mechanics, states depend in time while operators are time independent. In Heisenberg's picture the reverse happens. So, in Schrödinger's picture, this result holds for all operators of interest.*

End of Lecture 8

1.16 Observables and Hermitian Operators

Recall the definition of an Hermitian operator $\hat{Q}$.

Definition 1.3. ***(Hermitian Operator)***
We say that an operator $\hat{Q}$ is Hermitian if

$$(\Psi, \hat{Q}\Phi) := \int_{\mathbb{R}} \Psi^*\hat{Q}\Phi dx = \int_{\mathbb{R}} (\hat{Q}\Psi)^*\Phi dx =: (\hat{Q}\Psi, \Phi). \tag{1.154}$$

for any wavefunctions Ψ and Φ.

In this notation, the expectation value of Q becomes

$$\langle\hat{Q}\rangle_\Psi = \int_{\mathbb{R}} \Psi^*\hat{Q}\Psi dx = (\Psi, \hat{Q}\Psi). \tag{1.155}$$

From now on we consider $\hat{Q}$ to be Hermitian.

Proposition 1.2. *If $\hat{Q}$ is Hermitian, then $\langle\hat{Q}\rangle_\Psi \in \mathbb{R}$ for any wavefunction Ψ.*

Proof. Consider

$$\begin{aligned} (\langle\hat{Q}\rangle_\Psi)^* = (\Psi, \hat{Q}\Psi)^* &= \left(\int_{\mathbb{R}} \Psi^*\hat{Q}\Psi dx\right)^* \\ &= \int_{\mathbb{R}} \left(\Psi^*\hat{Q}\Psi\right)^* dx = \int_{\mathbb{R}} \Psi(\hat{Q}\Psi)^* dx \\ &= \int_{\mathbb{R}} (\hat{Q}\Psi)^*\Psi dx = (\hat{Q}\Psi, \Psi) = (\Psi, \hat{Q}\Psi) = \langle\hat{Q}\rangle_\Psi. \end{aligned} \tag{1.156}$$

■

Proposition 1.3. *If $\hat{Q}$ is Hermitian, its eigenvalues are real, i.e. if*

$$\hat{Q}\Psi_i = \lambda_i\Psi_i, \tag{1.157}$$

for Ψ_i an eigenstate of $\hat{Q}$, then $\lambda_i \in \mathbb{R}$.

Proof. We have

$$\langle \hat{Q} \rangle_{\Psi_i} = (\Psi_i, \hat{Q}\Psi_i) = (\Psi_i, \lambda_i \Psi_i) = \lambda_i (\Psi_i, \Psi_i) = \lambda_i, \tag{1.158}$$

therefore $\lambda_i \in \mathbb{R}$, assuming Ψ_i is normalized. If it is not, it is still a real number and the conclusion remains. ■

This also shows that when you measure a property of a normalized eigenstate with the action of an Hermitian operator the expectation value is precisely the eigenvalue.

Proposition 1.4. *Consider the collection of eigenfunctions and eigenvalues of the Hermitian operator $\hat{Q}$, i.e.*

$$\begin{aligned} \hat{Q}\Psi_1 &= q_1 \Psi_1 \\ \hat{Q}\Psi_2 &= q_2 \Psi_2 \\ &\vdots \end{aligned} \tag{1.159}$$

and assuming $q_i \neq q_j$. Then, the (normalized) eigenfunctions can be made pairwise orthogonal, i.e.

$$(\Psi_i, \Psi_j) = \int_{\mathbb{R}} \Psi_i^* \Psi_j dx = \delta_{ij}. \tag{1.160}$$

Proof. Consider

$$(\Psi_i, \hat{Q}\Psi_j) = q_j (\Psi_i, \Psi_j). \tag{1.161}$$

$$(\hat{Q}\Psi_i, \Psi_j) = q_i (\Psi_i, \Psi_j). \tag{1.162}$$

Then, since these are the same, we have

$$(q_i - q_j)(\Psi_i, \Psi_j) = 0, \tag{1.163}$$

since by assumption $q_i \neq q_j$, we conclude that $(\Psi_i, \Psi_j) = \delta_{ij}$. ■

Remark 1.13. *These proof is not complete since it may happen that different eigenfunctions have the same eigenvalue (called degeneracy). In this case, the eigenfunctions can still be transformed such that they are orthogonal. I suspect through a Gram-Schmidt process.*

Proposition 1.5. *The eigenfunctions of an Hermitian operator $\hat{Q}$ form a basis and therefore any wavefunction can be written as a linear combination (superposition) of eigenfunctions, i.e.*

$$\Psi(x) = \sum_i \alpha_i \Psi_i, \tag{1.164}$$

where Ψ_i are the eigenfunctions of $\hat{Q}$ and $\alpha_i \in \mathbb{C}$.

To compute the α_i we just need to project the state in the eigenstate, i.e.

$$\begin{aligned} (\Psi_i, \Psi) = \int_{\mathbb{R}} \Psi_i^* \Psi dx &= \int_{\mathbb{R}} \Psi_i^* \left(\sum_j \alpha_j \Psi_j \right) dx \\ &= \int_{\mathbb{R}} \left(\sum_j \alpha_j \Psi_i^* \Psi_j \right) dx = \sum_j \alpha_j \int_{\mathbb{R}} \Psi_i^* \Psi_j dx \\ &= \alpha_j \delta_{ij} = \alpha_i. \end{aligned} \tag{1.165}$$

Remark 1.14. *The commutation of the integral and the sum, if infinite, needs to be properly justified? It can be justified simply by linearity of the inner product for an Hilbert space?*

Furthermore, for a normalized state Ψ, we have

$$1 = \int_{\mathbb{R}} |\Psi|^2 dx = \int_{\mathbb{R}} \left(\sum_i \alpha_i \Psi_i \right)^* \left(\sum_j \alpha_j \Psi_j \right) dx = \sum_i \sum_j \alpha^i \alpha_j \int_{\mathbb{R}} \Psi_i^* \Psi_j dx = \sum_i |\alpha_i|^2. \tag{1.166}$$

Measurement Postulate: If we measure $\hat{Q}$ in the state Ψ, the possible outcomes are q_i with probability

$$p_i = |\alpha_i|^2 = |(\Psi_i, \Psi)|^2. \tag{1.167}$$

Note that this is true only if there is no degeneracy. After measuring the system, the state collapses into the state Ψ_i.

Example: Consider we have a state Ψ and we want to measure $\langle \hat{Q} \rangle$. We have

$$\begin{aligned} \langle \hat{Q} \rangle_\Psi = (\Psi, \hat{Q}\Psi) = \left(\sum_i \alpha_i \Psi_i, \hat{Q}(\sum_j \alpha_j \Psi_j) \right) = \sum_i \sum_j \alpha_i^* \alpha_j (\Psi_i, q_j \Psi_j) \\ = \sum_i \sum_j \alpha_i^* \alpha_j q_j \delta_{ij} = \sum_i |\alpha_i|^2 q_i. \end{aligned} \tag{1.168}$$

Which is consistent with the entire discussion. The average of the operator $\hat{Q}$ is just the average value of its possible values.

1.17 Uncertainty

The uncertainty is just the standard deviation ΔQ of the random variable Q. Thus, considering the possible values q_i with probability p_i we have

$$(\Delta Q)^2 = \sum_i p_i (q_i - \mathbb{E}(Q))^2 \geq 0. \tag{1.169}$$

Recalling that, for any random variable X we have

$$\mathbb{E}\left[(X - \bar{X})^2 \right] = \mathbb{E}[X^2] - (\mathbb{E}[X])^2. \tag{1.170}$$

Then, for Q we have

$$(\Delta Q)^2 = \mathbb{E}[Q^2] - (\mathbb{E}[Q])^2 \geq 0, \tag{1.171}$$

or equivalently

$$\mathbb{E}[Q^2] \geq (\mathbb{E}[Q])^2. \tag{1.172}$$

Therefore, given an operator $\hat{Q}$ in quantum mechanics, we define the uncertainty $\Delta \hat{Q}$ on the wavefunction Ψ as

$$(\Delta \hat{Q})^2_\Psi = \mathbb{E}[\hat{Q}^2]_\Psi - (\mathbb{E}[\hat{Q}])^2_\Psi := \langle \hat{Q}^2 \rangle - \langle \hat{Q} \rangle^2. \tag{1.173}$$

Proposition 1.6. *We have*

$$(\Delta\hat{Q})^2_\Psi = \langle(\hat{Q} - \langle\hat{Q}\rangle)^2\rangle \tag{1.174}$$

Proof. This is just the definition of variance from which we define the uncertainty, it's just the reverse of how we obtain it. ■

Proposition 1.7. *We have*

$$(\Delta\hat{Q})^2_\Psi = \int_{\mathbb{R}} \left|(\hat{Q} - \langle\hat{Q}\rangle)\Psi\right|^2 dx \tag{1.175}$$

Proof. Because $\hat{Q}$ is Hermitian we have that $(\hat{Q} - \mathbb{E}(\hat{Q}))$ is Hermitian since $\mathbb{E}(\hat{Q}) \in \mathbb{R}$. Therefore

$$\begin{aligned}(\Delta\hat{Q})^2_\Psi &= \int_{\mathbb{R}} \Psi^*(\hat{Q} - \mathbb{E}(\hat{Q})((\hat{Q} - \mathbb{E}(\hat{Q}))\Psi)) = \int_{\mathbb{R}} (\hat{Q} - \mathbb{E}(\hat{Q})\Psi)^*((\hat{Q} - \mathbb{E}(\hat{Q}))\Psi)) \\ &= \int_{\mathbb{R}} \left|(\hat{Q} - \langle\hat{Q}\rangle)\Psi\right|^2 dx.\end{aligned} \tag{1.176}$$

■

If Ψ is an eigenstate of $\hat{Q}$, i.e. $\hat{Q}\Psi = \lambda\Psi$, then

$$\langle\hat{Q}\rangle_\Psi = \lambda \int_{\mathbb{R}} \Psi^*\Psi dx = \lambda, \tag{1.177}$$

and thus

$$\hat{Q}\Psi = \langle\hat{Q}\rangle_\Psi \Psi. \tag{1.178}$$

Furthermore

$$(\Delta\hat{Q})^2_\Psi = \int_{\mathbb{R}} \left|(\hat{Q} - \langle\hat{Q}\rangle)\Psi\right|^2 dx = \int_{\mathbb{R}} |\lambda\Psi - \lambda\Psi|^2 = 0. \tag{1.179}$$

Thus, $(\Delta\hat{Q})^2_\Psi = 0$ iff Ψ is an eigenstate of $\hat{Q}$.

End of Lecture 9

2 Quantum Physics in 1D Potentials

2.1 Stationary Sates

Stationary states are not stationary in the usual sense, they may be time dependent. However, this time dependence takes a relatively simple form. In particular, we define a stationary state to be one where the time dependence and the spatial dependence can be factorized, i.e.

$$\Psi(x,t) = g(t)\psi(x), \tag{2.1}$$

where $\Psi(x,t)$ is a solution of Schrödinger's equation. In particular, we shall see that the expectation values of these (time-independent) observables are time-independent. This is not true in general since there is a time dependence on the expectation coming from the wavefunction itself.

Substituting $g(t)\psi(x)$ in Schrödinger's equation we get

$$i\hbar\psi(x)g'(t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right) g(t)\psi(x) \tag{2.2}$$

which leads to

$$i\hbar\psi(x)g'(t) = -\frac{\hbar^2}{2m}g(t)\psi''(x) + V(x)g(t)\psi(x) \tag{2.3}$$

and, separating variables and ignoring the trivial solution,

$$i\hbar\frac{g'(t)}{g(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) = \frac{1}{\psi(x)}\hat{H}\psi(x) = E, \tag{2.4}$$

with $E \in \mathbb{R}$, with units of energy (we will comment ahead why $E \in \mathbb{C}$ does not work).

Since this equation must hold for all x and t (independent variables) we conclude that they must equal a constant (e.g. for fixed t it must match all x which must then match for all t, i.e. they all take the same value). So, we get

$$i\hbar g'(t) = Eg(t), \tag{2.5}$$

with solution

$$g(t) = Ce^{-i\frac{E}{\hbar}t}, \tag{2.6}$$

$C \in \mathbb{C}$, and

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x), \tag{2.7}$$

or equivalently

$$\hat{H}\psi(x) = E\psi(x), \tag{2.8}$$

which is known as the time independent Schrödinger's equation (TISE). The full wavefunction is then

$$\Psi(x,t) = C\psi(x)e^{-i\frac{E}{\hbar}t}. \tag{2.9}$$

Let $C = 1$, if we normalize this state, we have

$$1 = \int_{\mathbb{R}} \Psi^*\Psi dx = \int_{\mathbb{R}} \psi^*(x)e^{i\frac{E}{\hbar}t}\psi(x)e^{-i\frac{E}{\hbar}t} = \int_{\mathbb{R}} |\psi(x)|^2, \tag{2.10}$$

and the time dependent term cancels out. On the other hand, had we chosen $E \in \mathbb{C}$, that would not be the case. We only need that the spatial part is normalized.

Let us compute the expectation of the Hamiltonian operator, which we expect should give us the energy.

$$\begin{aligned}
\langle \hat{H} \rangle_{\Psi(x,t)} &= \int_{\mathbb{R}} \psi^*(x) e^{i\frac{E}{\hbar}t} \hat{H} \left(\psi(x) e^{-i\frac{E}{\hbar}t} \right) dx \\
&= \int_{\mathbb{R}} \psi^*(x) e^{i\frac{E}{\hbar}t} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right) \left(\psi(x) e^{-i\frac{E}{\hbar}t} \right) dx \\
&= \int_{\mathbb{R}} \psi^*(x) \hat{H} \psi(x) dx \\
&= \langle \hat{H} \rangle_{\psi(x)} = E.
\end{aligned} \tag{2.11}$$

The Hamiltonian operator $\hat{H}$ does not act on the time dependence. Thus, the expectation of the Hamiltonian on the full stationary state is just the expectation on the spatial part of the stationary state. We make the following observations:

1. The expectation value of a time-independent operator $\hat{Q}$ in a stationary state is time independent.

$$\langle \hat{Q} \rangle_{\Psi(x,t)} = \int_{\mathbb{R}} \left(\Psi^*(x,t) \hat{Q} \Psi(x,t) \right) dx = \int_{\mathbb{R}} \psi^*(x) \hat{Q} \psi(x) = \langle \hat{Q} \rangle_{\psi(x)}. \tag{2.12}$$

2. The superposition (linear combination) of stationary states is not (necessarily) stationary. There's going to be mixed terms since, in general, the energies of the particles will be different.

Turning back to the TISE

$$\hat{H}\psi(x) = E\psi(x). \tag{2.13}$$

Since $\hat{H}$ is Hermitian, the eigenfunctions of $\hat{H}$ form a complete orthonormal set (as partially proved earlier, Props. 1.4 and 1.5). The eigenfunctions eigenvalue pairs $\{(\psi_1, E_1), (\psi_2, E_2), ...\}$ are called the spectrum of the theory. Rewriting the TISE we obtain

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} \left(V(x) - E \right) \psi(x). \tag{2.14}$$

Essentially, the potential function $V(x)$ dictates how bad this second order ODE is to solve.

- **Claim 1 (not rigorous):** $\psi(x) \in C^0(\mathbb{R})$.
  Suppose $\exists\, x_0 \in \mathbb{R}$ where ψ is discontinuous, then (in the sense of distributions) $\psi'(x_0)$ contains a delta function and $\psi''(x_0)$ a derivative of a delta function which does not appear on the RHS, where the worst case scenario is a delta-function.

- **Claim 2 (not rigorous):** $\psi'(x) \in C^0(\mathbb{R})$ unless $V(x)$ contains a delta-function.
  If $\psi' \notin C^1(\mathbb{R})$, then ψ'' is discontinuous and $V(x)$ on the RHS could be discontinuous, it's a possibility. On the other hand, if $\psi' \notin C^0(\mathbb{R})$, then ψ'' contains a delta-function which means that $V(x)$ must contain a delta-function.

2.2 Particle in a Circle

Consider a line $[0, L]$ and identify its two endpoints, i.e. $0 \leftrightarrow L$, equivalently $x \sim x + L$. This is topologically just S^1 (although not necessarily the circle). Consider the wavefunction on the circle which therefore satisfies

$$\psi(x + L) = \psi(x). \tag{2.15}$$

We consider $V(x) = 0$ such that

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}, \tag{2.16}$$

and we want to solve

$$\hat{H}\psi(x) = E\psi(x) \Leftrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x). \tag{2.17}$$

We multiply by ψ^* and integrate to obtain the following

$$\int_0^L \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}\right)dx = \int_0^L \psi^*(x)E\psi(x)dx = E. \tag{2.18}$$

Thus

$$\begin{aligned}
&= -\frac{\hbar^2}{2m}\left(\int_0^L \psi^*(x)\frac{d^2\psi(x)}{dx^2}dx\right) \\
&= -\frac{\hbar^2}{2m}\int_0^L \left(\frac{d}{dx}\left(\psi^*\frac{d\psi}{dx}\right) - \frac{d\psi^*}{dx}\frac{d\psi}{dx}\right)dx \\
&= -\frac{\hbar^2}{2m}\underbrace{\left(\psi^*(L)\frac{d\psi}{dx}(L) - \psi^*(0)\frac{d\psi}{dx}(0)\right)}_{=0} + \frac{\hbar^2}{2m}\int_0^L \left|\frac{d\psi}{dx}\right|^2 dx,
\end{aligned} \tag{2.19}$$

using the Fundamental Theorem of Calculus and periodicity of $\psi(x)$. So

$$E = \frac{\hbar^2}{2m}\int_0^L \left|\frac{d\psi}{dx}\right|^2 dx \geq 0. \tag{2.20}$$

However $E = 0 \implies d\psi(x)/dx = 0$, for all x, which means that ψ would be a constant function. So, we can write the TISE as

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x), \tag{2.21}$$

which is equivalent to

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x), \tag{2.22}$$

where $k = \sqrt{2mE}/\hbar \in \mathbb{R}$. The choice of the letter k is not arbitrary since $E = p^2/(2m) = \hbar^2k^2/(2m)$. The general solution of the above equation is just a linear combination of sines and cosines or complex exponential, therefore

$$\psi(x) = A\sin(kx) + B\cos(kx), \tag{2.23}$$

or

$$\psi(x) = Ae^{ikx}, \tag{2.24}$$

where $A, B \in \mathbb{C}$ are defined by the initial conditions. From the periodic condition we have

$$Ae^{ik(x+L)} = Ae^{ikx}, \tag{2.25}$$

which implies that $A = Ae^{ikL}$. If $A \neq 0$, then $e^{ikL} = 1$ and $k = 2n\pi/L$, for $n \in \mathbb{Z}$. We write $k_n = 2n\pi/L$, $n \in \mathbb{Z}$, where the sign defines in which direction the particle is traveling, counterclockwise if positive, clockwise if negative and stationary if $n = 0$. The momentum is given by $p = \hbar k_n = 2n\pi\hbar/L$ with energies $E = 2\pi\hbar^2 n^2/(mL^2)$. Normalizing we obtain

$$1 = \int_0^L |A|^2 dx = |A|^2 L, \tag{2.26}$$

and therefore $|A| = 1/\sqrt{L}$ or $A = 1/\sqrt{L}$, if we take it to be a real number. Thus, we conclude that the spatial part is

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{\frac{2\pi i n x}{L}} \tag{2.27}$$

and the full wavefunction is

$$\Psi_n(x,t) = \frac{1}{\sqrt{L}} e^{\frac{2\pi i n x}{L} - i\frac{E_n}{\hbar}t} \tag{2.28}$$

The $\Psi_{\pm j}(x,t)$, $j \in \mathbb{N}$, are degenerate states, they have the same energy $E_j = E_{-j}$, with different momentum and in particular

$$\hat{p}\psi_n(x) = p_n \psi_n(x). \tag{2.29}$$

These are orthonormal states since they are eigenfunctions of an Hermitian operator ($\hat{p}$) with different eigenvalues. By linearity, the most general wavefunction is a superposition

$$\psi(x) = \sum_{n\in\mathbb{Z}} a_n \psi_n(x), \tag{2.30}$$

$a_n \in \mathbb{C}$.

End of Lecture 10

2.3 Infinite Square Well

Consider the potential

$$V(x) = \begin{cases} \infty, & x \leq 0, \\ 0, & x \in (0,a), \\ \infty, & x \geq a. \end{cases} \tag{2.31}$$

Since it requires an infinite amount of energy to overcome an infinite potential barrier we have that $\psi(x) = 0$ for $x \leq 0$ or $x \geq a$ (or $x < 0$ or $x > a$ but then $\psi(0) = \psi(a) = 0$ by continuity). Again, the time-independent wavefunction satisfies

$$\psi'' = -\frac{2mE}{\hbar^2}\psi. \tag{2.32}$$

This time we consider the solution

$$\psi(x) = C_1 \cos(kx) + C_2 \sin(kx). \tag{2.33}$$

Since $\psi(0) = 0$, we have $C_1 = 0$. From $\psi(a) = 0$ we obtain

$$C_2 \sin(ka) = 0, \tag{2.34}$$

and therefore $C_2 = 0$, leading to the trivial solution, or $ka = n\pi$ for $n \in \mathbb{Z} \setminus \{0\}$, so $k_n = n\pi/a$. However, because $\sin(-x) = -\sin(x)$, leading to the same wavefunction, we should restrict $n \in \mathbb{N}$. If we normalize $\psi(x)$ we have

$$|C_2|^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1, \tag{2.35}$$

which we can integrate by parts twice, or use trigonometric relations, leading to

$$|C_2|^2 \frac{a}{2} = 1, \tag{2.36}$$

so $C_2 = \sqrt{2/a}$, and

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad n \in \mathbb{N}, \tag{2.37}$$

with energy

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}. \tag{2.38}$$

The ground state (state with lowest energy) corresponds to $n = 1$ and has no nodes, i.e. points $x \in (0, a)$ for which $\psi(x) = 0$. The numbers of nodes m, satisfies $m = n - 1$ (a general result for bound states, i.e. normalizable wave functions). If we consider $a = 2$ as the zero of a new system of coordinates we see that $\psi(x)$ is symmetric for odd n while it is antisymmetric for even n.

Proposition 2.1. *Bound states of a symmetric potential, $V(x) = V(-x)$, are either odd or even. Furthermore, there are no degenerate energy eigenstates for bound states of symmetrical potentials defined on the real line.*

Remark 2.1. *Classically, a particle contained in a potential well could have any continuous energy from its momentum. Here, because we must fit a wave that perfectly cancels at the end points of the well, this forces a quantization of the energy.*

2.4 Finite Square Well

Consider the potential

$$V(x) = \begin{cases} -V_0, & x \leq -a, \\ 0, & x \in (-a, a), \\ -V_0, & x \geq a, \end{cases} \tag{2.39}$$

with $V_0 > 0$. We are looking for bound states, i.e. the ones satisfying $E < 0$. The TISE is now given by

$$\psi'' = -\frac{2m}{\hbar^2} (E - V(x)) \psi. \tag{2.40}$$

Defining

$$\alpha := -\frac{2m}{\hbar^2} (E - V(x)), \tag{2.41}$$

we see that, taking $-V_0 < E < 0$ in $|x| < a$, then $E - V(x) > 0$ and $\alpha < 0$, i.e. we have trigonometric solutions for the TISE. For $|x| > a$, $\alpha > 0$ and the solutions are real exponentials. Using the previous proposition we either have even or odd solutions. We first look for **even solutions**, i.e. those satisfying

$$\psi(x) = \psi(-x), \tag{2.42}$$

for $|x| < a$. The TISE can be written as

$$\psi'' = -\frac{2m}{\hbar^2}\left(V_0 - |E|\right)\psi. \tag{2.43}$$

Define

$$k^2 = \frac{2m}{\hbar^2}\left(V_0 - |E|\right) > 0, \tag{2.44}$$

since $V_0 - |E| > 0$. We get then

$$\psi'' = -k^2\psi, \tag{2.45}$$

and the solution is

$$\psi(x) = \cos(kx). \tag{2.46}$$

In the $x > a$ region we have

$$\psi'' = \frac{2m}{\hbar^2}|E|\psi. \tag{2.47}$$

Define

$$\kappa^2 = \frac{2m}{\hbar^2}|E|, \tag{2.48}$$

the solution is then

$$\psi(x) = Ae^{-\kappa x}, \tag{2.49}$$

where we choose the $-$ sign in the exponential. Note that here we can not ignore the constant since we made a choice of norm for the wavefunction by not specifying a constant inside the well. They must match at the boundary. Now, we have

$$a^2(k^2 + \kappa^2) = \frac{2mV_0a^2}{\hbar^2}. \tag{2.50}$$

Define

$$\begin{cases} \xi = \kappa a > 0, \\ \eta = ka > 0, \end{cases} \tag{2.51}$$

which are unit free. We have

$$\xi^2 + \eta^2 = z_0^2 = \frac{2mV_0a^2}{\hbar^2}, \tag{2.52}$$

where, as we shall see, z_0 (adimensional) controls the number of bound states. We now match ψ at the boundary, by continuity, we have

$$\cos(ka) = Ae^{-\kappa a}. \tag{2.53}$$

By continuity of Ψ' we also have

$$-k\sin(ka) = -\kappa Ae^{-\kappa a}. \tag{2.54}$$

Dividing these equations, we obtain

$$\tan(ka) = \kappa/k. \tag{2.55}$$

Multiplying by a, we have

$$\eta\tan(\eta) = \xi. \tag{2.56}$$

Via the relations above we find also

$$\frac{|E|}{V_0} = \left(\frac{\xi}{z_0}\right)^2. \tag{2.57}$$

By plotting (2.52) and (2.56), their intersection gives the number of states and the possible values of the energy. See Fig. 1.

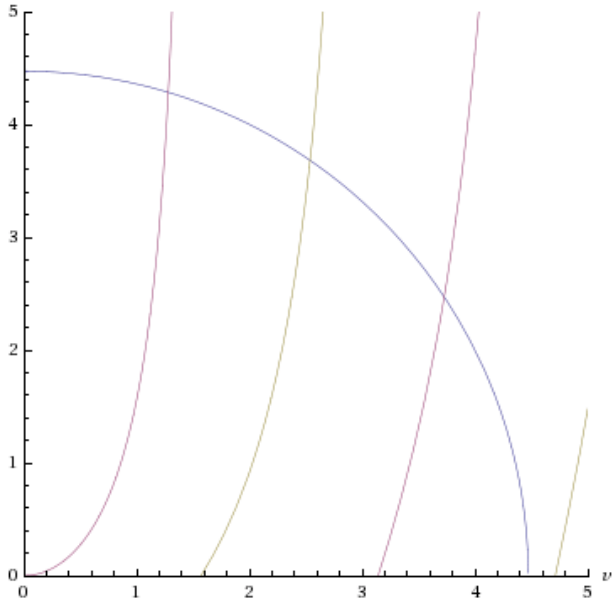

Figure 1: Plot of 2.52 and 2.56, the y axis corresponds to ξ and the x axis to η. The circle portion in the first quadrant has radius z_0. In this case we have 3 bound states.

By equation (2.57) we further realize that the state of largest value ξ corresponds to the state with largest energy while the state with largest η corresponds to the state with lowest energy. Also, we have always at least one state.

For the odd solutions, we have

$$\xi = -\eta \cot(\eta), \tag{2.58}$$

and there may be no such states if z_0 is small enough (to be done in the problem sets).

End of Lecture 11

2.5 Properties of Solutions

1. (Not proved) For 1D potentials over $x \in (-\infty, +\infty)$ there are no degenerate bound states, i.e. normalizable eigenstates where the wavefunction decays to zero when $x \to \pm\infty$.

2. With a real potential $V(x)$, the energy eigenstates can be chosen to be real. For 1D potentials, the bound states are real up to a phase.

   If $\psi(x) \in \mathbb{C}$ is a solution to the TISE, then $\psi^*(x)$ is also a solution with the same energy. Therefore we can consider $\psi_r(x) = 1/2(\psi(x) + \psi^*(x))$ or $\psi_{im}(x) = 1/(2i)(\psi(x) - \psi^*(x))$ as a real spatial wavefunction, where $\psi(x) = \psi_r(x) + i\psi_{im}(x)$.

However, for bound states, because there are no degenerate solutions, we must have $\psi_r(x) = C\psi_{im}(x)$, $C \in \mathbb{R}$. Thus

$$\psi(x) = \psi_r + i\psi_{im} = (1 + iC)\psi_r(x) = e^{i\text{Arg}(1+ic)}\sqrt{1+c^2}\psi_r(x). \tag{2.59}$$

3. If $V(x)$ is an even real potential, the energy eigenstates can be chosen to be even or odd under $x \to -x$. For 1D potentials, the bound states are either even or odd.

Proof. The differential equation is

$$\psi'' + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi = 0. \tag{2.60}$$

We check that $\varphi(x) = \psi(-x)$ also solve the TISE. We have

$$\varphi''(x) = \psi''(-x)(-1)^2 = \psi''(-x), \tag{2.61}$$

and, because $V(-x) = V(x)$, $\varphi(x)$ solves

$$\varphi(x) + \frac{2m}{\hbar^2}\left(E - V(x)\right)\varphi(x) = 0. \tag{2.62}$$

Remark 2.2. *To be completely explicit here. If we evaluate the TISE at $-x$, of course it still holds since it holds for all $x \in \mathbb{R}$. We are saying something different, we are saying that the function $\varphi(x)$, which is a complete reflection along the origin for $\psi(x)$, also satisfies the TISE. And this is only true because $V(x)$ is even.*

So, we can form symmetric and antisymmetric solutions with the same energy by taking following linear combinations

$$\begin{cases} \psi_{\text{s}}(x) = \frac{1}{2}(\psi(x) + \psi(-x)), \\ \psi_{\text{as}}(x) = \frac{1}{2}(\psi(x) - \psi(-x)). \end{cases} \tag{2.63}$$

This shows that we can choose even or odd solutions of the TISE for even potentials.

For bound states, considering real solutions, because there is no degeneracy it must be the case that

$$\psi(x) = C\psi(-x), \tag{2.64}$$

for some $C \in \mathbb{R}$. If we let $x \to -x$ we get

$$\psi(-x) = C\psi(x), \tag{2.65}$$

leading to

$$\psi(x) = C^2\psi(x), \tag{2.66}$$

and therefore $C = \pm 1$. If $C = 1$ we have

$$\psi(x) = \psi(-x), \tag{2.67}$$

and even solution. If $C = -1$ we have

$$\psi(x) = -\psi(-x), \tag{2.68}$$

an odd solution.

Remark 2.3. *This justifies why, in the symmetric square well, we can find solutions by looking at either even or odd solutions, because there are no other solutions.*

■

2.6 Qualitative insights into (real) energy eigenstates:

General goal: Obtain qualitative insights on the wavefunction without explicitly solving Schrödinger's equation, which may be quite hard depending on the potential.

Wavelength behaviour: We have $E = K(x) + V(x)$ and we should expect the wavelength to corresponds to de Broglie's wavelength (which motivated the entire thing), i.e. $E = p^2/2m$ and $\lambda = \hbar/p(x)$, which is exactly true for a constant potential. For a general $V(x)$, as V increases, K decreases and therefore p decreases and λ increases, this is approximately true, the actual relations must be obtained by solving Schrödinger's equation.

Correspondence principle (amplitude behaviour): Vaguely, it states that the probability $|\Psi(x)|^2 dx$, and thus the amplitude of the wavefunction, of finding a particle in $[x, x+dx]$ is proportional to the time the particle spends in that interval, i.e. dt/T, where T is the period. Since $dt/T = dx/(v(x)T)$, we have

$$|\Psi(x)|^2 dx \propto dt/T = \frac{dx}{v(x)T} = \frac{mdx}{p(x)T}, \tag{2.69}$$

thus

$$|\Psi(x)|^2 \propto \frac{1}{p(x)} = \frac{\lambda(x)}{\hbar}, \tag{2.70}$$

and ultimately

$$|\Psi(x)| \propto \sqrt{\lambda(x)}. \tag{2.71}$$

Local behaviour: Let's write the TISE in the following way

$$\frac{1}{\psi}\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - V(x)\right). \tag{2.72}$$

- (A) $E - V(x) < 0$ corresponds to the classically forbidden region where the RHS> 0. Either
  1. $\psi > 0$ and thus also $d^2\psi/dx^2 > 0$.
  2. $\psi < 0$ and thus also $d^2\psi/dx^2 < 0$.

  Giving us a relation of concavity and the sign of ψ.
- (B) $E - V(x) > 0$ corresponds to the classically allowed region where the RHS< 0. Either
  1. $\psi > 0$ and thus also $d^2\psi/dx^2 < 0$.
  2. $\psi < 0$ and thus also $d^2\psi/dx^2 > 0$.
- (C) $E - V(x_0) = 0$ corresponds to turning points, where, if $\psi(x_0) \neq 0$, then

$$\frac{d^2\psi(x_0)}{dx^2} = 0, \tag{2.73}$$

and x_0 is an inflection point. When $\psi = 0$, from

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - V(x)\right)\psi, \tag{2.74}$$

we automatically get inflection points at the nodes.

End of Lecture 12

2.7 Delta function Potential

We now consider a delta function potential, i.e.

$$V(x) = -\alpha\delta(x), \;\; \alpha > 0. \tag{2.75}$$

Before jumping to the differential equation let us try to guess how the possible bound state energies look like via dimensional analysis. We have three constants in the problem, α, $\hbar$ and m. Since $\delta(x)$ integrates to 1, we have $[\delta(x)] = 1/L$ and therefore

$$[E] = \frac{[\alpha]}{L}. \tag{2.76}$$

From $E = p^2/2m$ and $p = \hbar/\lambda$ we further have

$$[E] = \frac{[\alpha]}{L} = \frac{[\hbar]^2}{ML^2}, \tag{2.77}$$

which leads to

$$L = \frac{[\hbar]^2}{[\alpha]M}. \tag{2.78}$$

Using again $E = \frac{[\hbar]^2}{ML^2}$, with this L, we finally get

$$E = M\frac{[\alpha]^2}{[\hbar]^2}. \tag{2.79}$$

Thus, the unique way to obtain the energy from this constants is of the form

$$E = -\#m\frac{\alpha^2}{\hbar^2}, \tag{2.80}$$

for some possible constants $\# > 0$. Now, in the region where $x \neq 0$, the TISE is given by

$$\psi'' = k^2\psi, \tag{2.81}$$

where

$$k^2 = -\frac{2mE}{\hbar^2} \geq 0, \tag{2.82}$$

leading to solutions of the form

$$e^{kx}, \;\; e^{-kx}, \;\; \sinh(x), \;\; \cosh(x). \tag{2.83}$$

Since the potential is even, the ground state is even and parity alternates. Thus, the first excited state would have to be odd and therefore $\psi(0) = 0$. The only possible solution of this form is $\sinh(x)$ which blows-up as $x \to \pm\infty$. Thus, we conclude that there can be no excited states and we will have a ground state, at most (they must alternate parity as we have seen before).

The only possible solution for a bound state (which decays at infinity) is of the form

$$\psi(x) = Ae^{-k|x|} = \begin{cases} Ae^{-kx}, & x > 0, \\ Ae^{kx}, & x < 0, \end{cases} \tag{2.84}$$

with ψ continuous but ψ' discontinuous at $x = 0$. We now use the delta function information to determine the type of discontinuity. At $x = 0$ we have

$$-\frac{\hbar^2}{2m}\psi'' - \alpha\delta(x)\psi = E\psi, \tag{2.85}$$

and we integrate from $-\epsilon$ to ϵ

$$\int_{-\epsilon}^{\epsilon} \left(-\frac{\hbar^2}{2m}\psi'' - \alpha\delta(x)\psi\right) dx = \int_{-\epsilon}^{\epsilon} (E\psi)\, dx, \tag{2.86}$$

leading to

$$-\frac{\hbar^2}{2m}\left(\psi'(\epsilon) - \psi'(-\epsilon)\right) - \alpha\psi(0) = \int_{-\epsilon}^{\epsilon} (E\psi)\, dx. \tag{2.87}$$

We now take the limit as $\epsilon \to 0$ obtaining

$$\lim_{\epsilon\to 0} -\frac{\hbar^2}{2m}\left(\psi'(\epsilon) - \psi'(-\epsilon)\right) - \alpha\psi(0) = 0, \tag{2.88}$$

where the RHS vanishes since ψ is continuous. We write this as

$$\Delta_0\psi' = -\frac{2m\alpha}{\hbar^2}\psi(0), \tag{2.89}$$

where Δ_0 represents the discontinuity in ψ' at $x = 0$. From the previous solution we obtain

$$\lim_{\epsilon\to 0}\left(-kAe^{-k\epsilon} - kAe^{-k\epsilon}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0), \tag{2.90}$$

and therefore

$$kA = \frac{m\alpha}{\hbar^2}A, \tag{2.91}$$

since $\psi(0) = A$ by continuity, and therefore

$$k = \frac{m\alpha}{\hbar^2}. \tag{2.92}$$

We obtain then

$$E = -\frac{k^2\hbar^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}, \tag{2.93}$$

which matches our initial guess.

2.8 Node Theorem (Intuitive Argument)

The statement is: given $\psi_1, \psi_2, ...$ bound energy eigenstates of a 1D potential with $E_1 < E_2 < ...$, ψ_n has $n - 1$ nodes.

For the square-well we haver shown this by explicitly computing all the energy eigenstates, we now argue that this is true for an arbitrary potential. We further use the fact that

$$\psi(x_0) = \psi'(x_0) = 0, \tag{2.94}$$

can not happen. We turn an arbitrary potential $V(x)$ into a screened potential (square-well potential) given by

$$V_a(x) = \begin{cases} V(x), & |x| < a, \\ \infty, & |x| > a. \end{cases} \tag{2.95}$$

The idea then is that the bound states as $a \to \infty$ are the bound states of $V(x)$. If we take a small, we can consider that the potential is symmetric, since it will be flat, and thus our energy eigenstates satisfy the node Theorem as seen before. We now argue that, as we increase a, we can not possibly increase the number of nodes continuously, since we are assuming that the bound states vary continuously when varying a.

Consider a bound eigenstate with n nodes for a potential with width a_1. Could it be that increasing to $a_2 > a_1$ the same eigenstate could have an extra node? Drawing this, it is clear that $\psi'(a_1) < 0$ and $\psi'(a_2) > 0$ (or vice-versa) and therefore, there exists some width a satisfying $a_1 < a < a_2$ such that $\psi(a) = \psi'(a) = 0$, by continuity. This however contradicts the fact above and therefor argues that it not possible for the number of nodes to change.

2.9 Simple Harmonic Oscillator

The energy of the classical simple harmonic oscillator is given by $E = p^2/2m + 1/2m\omega^2 x^2$, where $\omega = \sqrt{k/m}$, k the spring constant. The quantum case considers the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \tag{2.96}$$

where

$$[\hat{x}, \hat{p}] = i\hbar. \tag{2.97}$$

The extremum of any potential can be approximated by a quadratic potential by Taylor approximation, which makes the harmonic oscillator a very useful system in approximating other potentials.

We want to solve

$$\hat{H}\varphi(x) = E\varphi(x), \tag{2.98}$$

or

$$-\frac{\hbar^2}{2m}\varphi''(x) + \frac{1}{2}m\omega^2 x^2\varphi(x) = E\varphi(x). \tag{2.99}$$

First, we want to make this unit free, which we do by considering

$$x = au, \tag{2.100}$$

where u is unit free and $[a] = L$. Thus, by dimensional analysis, using the constants of the problem $(\omega, \hbar, m)$, we have

$$a = m^\alpha \omega^\beta \hbar^\gamma = M^{\alpha+\gamma} T^{-\beta-\gamma} L^{2\gamma}, \tag{2.101}$$

leading to $\alpha = -1/2$, $\beta = -1/2$ and $\gamma = 1/2$, such that

$$a^2 = \frac{\hbar}{m\omega}. \tag{2.102}$$

Temporarily, consider $\varphi(x) = (f \circ u)(x)$. Writing the TISE for f we obtain

$$-\frac{\hbar^2}{2ma^2} f''(u) + \frac{1}{2} m\omega^2 a^2 u^2 f(u) = Ef(u), \tag{2.103}$$

since

$$\frac{d\varphi}{dx}(x) = \frac{df}{du}(u(x))\frac{du}{dx}(x) = \frac{1}{a}\frac{df}{du}(u). \tag{2.104}$$

We now rename f as φ again such that

$$-\frac{\hbar^2}{2ma^2} \varphi''(u) + \frac{1}{2} m\omega^2 a^2 u^2 \varphi(u) = E\varphi(u), \tag{2.105}$$

using the definition of a we now get

$$-\frac{1}{2}\hbar\omega\varphi''(u) + \frac{1}{2}\hbar\omega u^2 \varphi(u) = E\varphi(u), \tag{2.106}$$

and multiplying by $2/(\hbar\omega)$ we get

$$-\varphi''(u) + u^2\varphi(u) = \epsilon\varphi(u), \tag{2.107}$$

where

$$\epsilon = \frac{2E}{\hbar\omega}, \tag{2.108}$$

is a unit free "energy". We can finally write this as

$$\varphi''(u) = (u^2 - \epsilon)\varphi(u). \tag{2.109}$$

Remark 2.4. *Not introducing f is sloppy and rather confusing.*

When $u \to \pm\infty$ we have

$$\varphi''(u) \approx u^2\varphi(u). \tag{2.110}$$

In this region, the solutions can be written as $u^k e^{(\alpha/2)u^2}$ since

$$\varphi''(u) = (\alpha u)^2\varphi(u) + \text{subleading terms}. \tag{2.111}$$

The point of the u^k term is that when we differentiate we get $u^q e^{\alpha/2u^2}$ terms where $q < k$. This will diverge more slowly than the exponential term so it will change nothing in the limit. We have then $\alpha = \pm 1$ and solutions at infinity are of the form

$$\varphi(x) \approx Au^k e^{-u^2/2} + Bu^k e^{u^2/2}, \tag{2.112}$$

where we want $B = 0$ to obtain normalizable states. We propose then the ansatz

$$\varphi(u) = h(u)e^{-u^2/2}, \tag{2.113}$$

without loss of generality since $e^{-u^2/2}$ is a scale factor capturing the behavior we want at infinity, depending on $h(u)$. Obtaining the differential equation for $h(u)$ by substituting back we have

$$h''(u) - 2uh'(u) + (\epsilon - 1)h(u) = 0. \tag{2.114}$$

End of Lecture 13

We attempt a series expansion solution to equation (2.114). Suppose

$$h(u) = \sum_{k=0}^{\infty} a_k u^k. \tag{2.115}$$

To find the substituted equation we look at each power $a_j u^j$ appearing on the LHS. We have the following:

- The term $h''(u)$ of order u^j must come from differentiating $a_{j+2}u^{j+2}$, resulting in $a_{j+2}(j+2)(j+1)u^j$.
- The term $-2uh'(u)$ of order u^j must come from differentiating $a_j u^j$, resulting in $-2ja_j u^j$.
- The term $(\epsilon - 1)h(u)$ is simply $(\epsilon - 1)a_j u^j$.

Thus, the u^j term has the following form

$$\left[a_{j+2}(j+2)(j+1) - 2ja_j + (\epsilon - 1)a_j\right] u^j. \tag{2.116}$$

Summing all terms we get the following equation

$$\sum_{k=0}^{\infty} \left[a_{k+2}(k+2)(k+1) - 2ka_k + (\epsilon - 1)a_k\right] u^k = 0. \tag{2.117}$$

Since, for all u, the powers u^k form a linearly independent basis we must have

$$a_{k+2}(k+2)(k+1) - 2ka_k + (\epsilon - 1)a_k = 0, \tag{2.118}$$

leading to the recursion relation

$$a_{k+2} = \frac{(2k + 1 - \epsilon)}{(k+2)(k+1)} a_k. \tag{2.119}$$

Thus, given a_0 we know $a_2, a_4, a_6, ...$, i.e. the even powered solutions. Given a_1 we know $a_3, a_5, a_7, ...$, i.e. the odd powered solutions. Note that $a_0 = h(0)$ and $a_1 = h'(0)$ are the initial data for the second order ODE for h. We observe that the coefficients when $k \to \infty$ decay as

$$\lim_{k\to\infty} \frac{a_{k+2}}{a_k} \approx \lim_{k\to\infty} \frac{2}{k}. \tag{2.120}$$

We now guess a coefficient a_k satisfying this behavior. Note that

$$e^{u^2} = \sum_{n=0}^{\infty} \frac{1}{n!} u^{2n} = \sum_{j=0,2,...} \frac{1}{(j/2)!} u^j. \tag{2.121}$$

Defining

$$a_k := \frac{u^k}{(k/2)!}, \;\; k = 2j, \;\; j \in \mathbb{N}_0, \tag{2.122}$$

we have

$$\frac{a_{k+2}}{a_k} = \frac{\left(\frac{k}{2}\right)!}{\left(\frac{k+2}{2}\right)} = \frac{2}{k}, \tag{2.123}$$

which has the decay we are looking for for large k. However, if the series does not truncate, i.e. stops at a certain finite number of terms, for $h(u) = e^{u^2}$ it will diverge, since $e^{u^2} e^{-u^2/2} = e^{u^2/2}$. This is not normalizable and therefore is not a physical solution. Thus, for the series to truncate, there must exist k such that $2k + 1 = \epsilon$, from equation (2.119), and thus $a_{k+2} = 0$. We can write then

$$h(u) = a_j u^j + a_{j-2} u^{j-2} + ..., \tag{2.124}$$

letting $j = n$, we have the adimensional energies

$$\epsilon_n = 2n + 1, \tag{2.125}$$

and

$$h(u) = a_n u^n + a_{n-2} u^{n-2} + ..., \;\; n \in \mathbb{N}_0, \tag{2.126}$$

with actual energies

$$E_n = \hbar\omega(n + 1/2). \tag{2.127}$$

Substituting $\epsilon_n = 2n + 1$ in the starting equation we obtain

$$H_n''(u) - 2uH_n'(u) + 2nH_n(u) = 0, \tag{2.128}$$

which is called Hermite's polynomial equation, with Hermite polynomials usually written as

$$H_n(u) = 2^n u^n + ...u^{n-2} + ..., \tag{2.129}$$

such that

$$\begin{aligned} H_0 &= 1, \\ H_1 &= 2u, \\ H_2 &= 4u^2 - 2, \\ H_3 &= 8u^3 - 12u, \\ &\vdots \end{aligned} \tag{2.130}$$

Returning to the original variable $x = ua$, we have the eigenstates

$$\varphi_n(x) = N_n H_n(x/a) e^{-\frac{x^2}{2a^2}} = N_n H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{m\omega}{2\hbar}x^2}, \tag{2.131}$$

where N_n is some normalization constant.

2.10 Simple Harmonic Oscillator (Algebraic Version)

We notice that

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \frac{m\omega^2}{2}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right). \tag{2.132}$$

We want to factorize the Hamiltonian as $\hat{H} = V^\dagger V + \#$ (this form makes it an Hermitian operator), for some factor V and number $\#$ (the number simply shifts the energies). If we let

$$V = \hat{x} + \frac{i}{m\omega}\hat{p}, \tag{2.133}$$

then

$$V^\dagger V = \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} + \frac{i}{m\omega}[\hat{x}, \hat{p}] = \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} - \frac{\hbar}{m\omega}, \tag{2.134}$$

thus

$$\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} = \left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) + \frac{\hbar}{m\omega}. \tag{2.135}$$

Thus,

$$\hat{H} = \frac{m\omega^2}{2} V^\dagger V + \frac{\hbar\omega}{2}. \tag{2.136}$$

We have

$$[V, V^\dagger] = -\frac{i}{m\omega}[\hat{x}, \hat{p}] - \frac{i}{m\omega}[\hat{p}, \hat{x}] = \frac{2\hbar}{m\omega}, \tag{2.137}$$

therefore

$$\left[\sqrt{\frac{m\omega}{2\hbar}} V, \sqrt{\frac{m\omega}{2\hbar}} V^\dagger\right] = 1. \tag{2.138}$$

We define now

$$\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}} V = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \tag{2.139}$$

$$\hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}} V^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega}\hat{p}\right), \tag{2.140}$$

such that

$$\hat{x} = \sqrt{\frac{2\hbar}{m\omega}} \left(\frac{\hat{a} + \hat{a}^\dagger}{2}\right), \tag{2.141}$$

and

$$\hat{p} = i\sqrt{\frac{2\hbar}{m\omega}} \left(\frac{\hat{a}^\dagger - \hat{a}}{2}\right), \tag{2.142}$$

are Hermitian operators. We can then write the Hamiltonian as

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right). \tag{2.143}$$

The expected value in a normalized state Ψ is given by

$$\begin{aligned} \left\langle \hat{H} \right\rangle_\Psi &= \left\langle \Psi, \hbar\omega \hat{a}^\dagger \hat{a} \Psi + \frac{\hbar\omega}{2} \Psi \right\rangle = \frac{\hbar\omega}{2} \langle \Psi, \Psi \rangle + \hbar\omega \left\langle \Psi, \hat{a}^\dagger \hat{a} \Psi \right\rangle \\ &= \frac{\hbar\omega}{2} + \hbar\omega \langle \hat{a}\Psi, \hat{a}\Psi \rangle \geq \frac{\hbar\omega}{2}, \end{aligned} \tag{2.144}$$

since

$$\langle \hat{a}\Psi, \hat{a}\Psi \rangle \geq 0. \tag{2.145}$$

Thus, if there is a ground state Ψ_0 such that we have exactly

$$\left\langle \hat{H} \right\rangle_{\Psi_0} = \frac{\hbar\omega}{2}, \tag{2.146}$$

then it must necessarily be the case that

$$\hat{a}\Psi_0 = 0, \tag{2.147}$$

giving $\hat{a}$ the name of annihilation operator. This means

$$\sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \Psi_0 = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right) \Psi_0(x) = 0, \tag{2.148}$$

reducing the starting second order differential equation into a first order differential equation. Equivalently we have

$$\frac{1}{\Psi_0}\frac{d\Psi_0}{dx} = -\frac{m\omega}{\hbar} x. \tag{2.149}$$

Integrating the above equation in x leads to

$$\Psi_0(x) = N_0 e^{-\frac{m\omega}{2}x^2}, \tag{2.150}$$

where the normalization constant N_0 is

$$N_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}, \tag{2.151}$$

which we can confirm by computing

$$\hat{H}\Psi_0 = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\Psi_0 = \frac{\hbar\omega}{2}\Psi_0. \tag{2.152}$$

From the commutation relation for $\hat{a}$ and $\hat{a}^\dagger$ we have

$$\hat{1}\Psi_0 = [\hat{a}, \hat{a}^\dagger]\Psi_0 = (\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a})\Psi_0 = \hat{a}\hat{a}^\dagger\Psi_0 = \Psi_0, \tag{2.153}$$

which means that $\hat{a}^\dagger\Psi_0$ does not destroy the state.

End of Lecture 14

Define the **number operator** $\hat{N}$ as

$$\hat{N} = \hat{a}^\dagger\hat{a}, \tag{2.154}$$

which encodes the Hamiltonian $\hat{H}$. We now look at a few commutators which will be useful. We have

$$[\hat{N}, \hat{a}] = [\hat{a}^\dagger\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}]\hat{a} = -\hat{a}, \tag{2.155}$$

$$[\hat{N}, \hat{a}^\dagger] = [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger, \tag{2.156}$$

and

$$[\hat{a}, (\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^{k-1}, \tag{2.157}$$

$$[\hat{a}^\dagger, \hat{a}^k] = -k\hat{a}^{k-1}, \tag{2.158}$$

where we use the commutator of $[\hat{a}, \hat{a}^\dagger] = 1$ to compute the last two results. We can further compute

$$[\hat{N}, \hat{a}^k] = -k\hat{a}^k, \tag{2.159}$$

$$[\hat{N}, (\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^k, \tag{2.160}$$

these last two relations is why one calls $\hat{N}$ the number operator.
Let us now consider the state

$$\varphi_1 = \hat{a}^\dagger\varphi_0, \tag{2.161}$$

which we which to check if it is an energy eigenstate (or a number eigenstate equivalently), we have

$$\hat{N}\varphi_1 = \hat{a}^\dagger\hat{a}\hat{a}^\dagger\varphi_0 = [\hat{N}, \hat{a}^\dagger]\varphi_0 = \varphi_1, \tag{2.162}$$

confirming that φ_1 is indeed an eigenstate of $\hat{N}$ with eigenvalue 1 and thus the state as energy

$$E_1 = \frac{3}{2}\hbar\omega, \tag{2.163}$$

recalling that $\hat{H} = \hbar\omega(\hat{N} + 1/2)$. Because of this property $\hat{a}^\dagger$ is called the creation operator (or raising operator). Starting under the assumption that φ_0 is normalized we check

$$\|\varphi_1\|^2 = (\hat{a}^\dagger\varphi_0, \hat{a}^\dagger\varphi_0) = (\varphi_0, \hat{a}\hat{a}^\dagger\varphi_0) = (\varphi_0, \varphi_0 + \hat{a}^\dagger\hat{a}\varphi_0) = (\varphi_0, \varphi_0) = 1, \tag{2.164}$$

using the commutator relation. We now check if the next state is an eigenstate of the energy

$$\hat{N}\varphi_2' = \hat{a}^\dagger\hat{a}(\hat{a}^\dagger)^2\varphi_0 = [\hat{N},(\hat{a}^\dagger)^2]\varphi_0 = 2(\hat{a}^\dagger)^2\varphi_0 = 2\varphi_2'. \tag{2.165}$$

It is also normalized since

$$\begin{aligned}\|\varphi_2'\|^2 &= (\hat{a}^\dagger\hat{a}^\dagger\varphi_0, \hat{a}^\dagger\hat{a}^\dagger\varphi_0) = (\varphi_0, \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger\varphi_0) = (\varphi_0, \hat{a}(1+\hat{a}^\dagger\hat{a})\hat{a}^\dagger\varphi_0)\\ &= (\varphi_0, \hat{a}\hat{a}^\dagger\varphi_0 + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger\varphi_0) = (\varphi_0, \hat{a}\hat{a}^\dagger\varphi_0 + \hat{a}\hat{a}^\dagger(1+\hat{a}^\dagger\hat{a})\varphi_0)\\ &= (\varphi_0, 2\hat{a}\hat{a}^\dagger\varphi_0) = 2(\varphi_0,\varphi_0) = 2,\end{aligned} \tag{2.166}$$

which can be computed much faster using the commutator relations. Thus, defining

$$\varphi_2 = \frac{1}{\sqrt{2}}(\hat{a}^\dagger)^2\varphi_0, \tag{2.167}$$

then the state is properly normalized. In general then, the n^{th} excited state is given by

$$\varphi_n = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\varphi_0, \tag{2.168}$$

with

$$\hat{N}\varphi_n = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\varphi_0 = \frac{1}{\sqrt{n!}}[\hat{N},(\hat{a}^\dagger)^n]\varphi_0 = n\varphi_n, \tag{2.169}$$

which is an energy eigenstate with eigenvalue n and therefore the energy is

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right). \tag{2.170}$$

We can further confirm is it properly normalized by computing

$$(\varphi_n,\varphi_n) = \frac{1}{n!}(\varphi_0, \hat{a}^n(\hat{a}^\dagger)^n\varphi_0) = \frac{1}{n!}(\varphi_0, \hat{a}^n(\hat{a}^\dagger)^n\varphi_0) = \frac{n(n-1)}{n!}(\varphi_0, (\hat{a})^{n-2}(\hat{a}^\dagger)^n\varphi_0) = 1. \tag{2.171}$$

To finalize we check what the lowering (or destruction) operator $\hat{a}$ and the creation (or raising) operator does to φ_n. We have

$$\begin{aligned}\hat{a}\varphi_n &= \frac{1}{\sqrt{n!}}\hat{a}(\hat{a}^\dagger)^n\varphi_0 = \frac{1}{\sqrt{n!}}[\hat{a},(\hat{a}^\dagger)^n]\varphi_0\\ &= \frac{n}{\sqrt{n!}}(\hat{a}^\dagger)^{n-1}\varphi_0 = \frac{n\sqrt{(n-1)!}}{\sqrt{n!}}\varphi_{n-1}\\ &= \sqrt{n}\varphi_{n-1}.\end{aligned} \tag{2.172}$$

Similarly,

$$\hat{a}^\dagger\varphi_n = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^{n+1}\varphi_0 = \sqrt{\frac{(n+1)!}{n!}}\varphi_{n+1} = \sqrt{n+1}\varphi_{n+1}. \tag{2.173}$$

Remark 2.5. *The algebraic method does not show that the ground state φ_0 is realizable, it proceeds under the assumption that it is. Furthermore, it assumes the next excited state φ_1 is of the form $\hat{a}^\dagger\varphi_0$, and so on.*

Example: Compute the following expectation values

$$\langle\hat{x}\rangle_{\varphi_n} = \int_{\mathbb{R}} x\varphi_n^2 dx = 0, \tag{2.174}$$

since φ_n is either even or odd and therefore φ_n^2 is even and $x\varphi_n^2$ is odd.

$$\langle \hat{p} \rangle_{\varphi_n} = 0, \tag{2.175}$$

since these are stationary states. We can also compute this by explicitly writing $\hat{x}$ and $\hat{p}$ as functions of $\hat{a}$ and $\hat{a}^\dagger$ and use the fact that

$$(\varphi_n, \varphi_m) = \delta_{nm}. \tag{2.176}$$

Without loss of generality let $n > m$ then this can be seen explicitly by computing

$$(\varphi_n, \varphi_m) \propto ((\hat{a}^\dagger)^n \varphi_0, (\hat{a}^\dagger)^m \varphi_0) = (\varphi_0, \hat{a}^n (\hat{a}^\dagger)^m \varphi_0) = 0. \tag{2.177}$$

In any case, we have already proven that eigenstates of Hermitian operators are orthogonal. We now compute

$$\begin{aligned}
(\Delta x)_{\varphi_n} = \left\langle x^2 \right\rangle_{\varphi_n} &= \int_{\mathbb{R}} x^2 \varphi_n^2 dx = \frac{2\hbar}{m\omega} \left(\varphi_n, \left(\frac{\hat{a} + \hat{a}^\dagger}{2} \right)^2 \varphi_n \right) \\
&= \frac{\hbar}{2m\omega} \left(\varphi_n, \left(\hat{a}^\dagger \hat{a}^\dagger + \hat{a}\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} \right) \varphi_n \right) \\
&= \frac{\hbar}{2m\omega} \left(\varphi_n, \left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} \right) \varphi_n \right) \\
&= \frac{\hbar}{2m\omega} \left(\varphi_n, \left([\hat{a}, \hat{a}^\dagger] + \hat{a}^\dagger \hat{a} + \hat{N} \right) \varphi_n \right) \\
&= \frac{\hbar}{2m\omega} \left(\varphi_n, \left(1 + 2\hat{N} \right) \varphi_n \right) \\
&= \frac{\hbar}{2m\omega} (1 + 2n) \left(\varphi_n, \varphi_n \right) \\
&= \frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right).
\end{aligned} \tag{2.178}$$

In the problem sheet we further compute $(\Delta \hat{p})_{\varphi_n}$ and $(\Delta x \Delta p)_{\varphi_n}$.

2.11 Scattering States

Scattering states are non-normalizable energy eigenstates, each individually can not represent a particle but an infinite sum of then can. We start by analyzing the step potential given by

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & x \leq 0. \end{cases} \tag{2.179}$$

Let us first consider the case where $E > V_0$ and imagine the wave moving from the left ($x < 0$) to the right ($x > 0$) (one can also consider the reverse scenario). As we have seen already, we have

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0, \\ Ce^{i\bar{k}x}, x > 0, \end{cases} \tag{2.180}$$

where $k^2 = 2mE/\hbar^2$ and $\bar{k}^2 = 2m(E - V_0)/\hbar^2$. By continuity of the wavefunction and its derivative, respectively, we further have

$$A + B = C \tag{2.181}$$

and

$$ikA - ikB = i\bar{k}C, \tag{2.182}$$

or rather

$$A - B = C\frac{\bar{k}}{k}. \tag{2.183}$$

We consider A the amount of incoming wave, which we usually fix to be equal to one, and we want to obtain the reflected proportion and the transmitted proportion. Respectively, they are

$$\frac{B}{A} = \frac{k - \bar{k}}{k + \bar{k}}, \tag{2.184}$$

and

$$\frac{C}{A} = \frac{2k}{k + \bar{k}}. \tag{2.185}$$

This is however not the full story since these wavefunctions can not be interpreted as physical particles since they are not normalizable.

End of Lecture 15

We now use conservation of probability current. Recall that

$$J(x) = \frac{\hbar}{m}\mathrm{Im}\left(\Psi^* \frac{\partial \Psi}{\partial x}\right). \tag{2.186}$$

For $x < 0$, we have

$$J_L(x) = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right), \tag{2.187}$$

while for $x > 0$, we have

$$J_R(x) = \frac{\hbar \bar{k}}{m}|C|^2. \tag{2.188}$$

which should be equal constants. In particular we have

$$\begin{aligned} J_L &= \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) = \frac{\hbar k}{m}\left(1 - \frac{|B|^2}{|A|^2}\right)|A|^2 = \frac{\hbar k}{m}\left(1 - \frac{(k-\bar{k})^2}{(k+\bar{k})^2}\right)|A|^2 \\ &= \frac{\hbar \bar{k}}{m}\left(\frac{2k}{k+\bar{k}}\right)^2 |A|^2 = \frac{\hbar \bar{k}}{m}|C|^2, \end{aligned} \tag{2.189}$$

i.e.

$$J_L = J_R. \tag{2.190}$$

We can further write

$$J_L = J_A - J_B, \tag{2.191}$$

where

$$J_A = \frac{\hbar k}{m}|A|^2, \tag{2.192}$$

and

$$J_B = \frac{\hbar k}{m}|B|^2. \tag{2.193}$$

From this, we define the reflection coefficient as

$$R := \frac{J_B}{J_A} = \left|\frac{B}{A}\right|^2, \tag{2.194}$$

and the transmission coefficient as

$$T := \frac{J_C}{J_A} = \frac{\bar{k}}{k}\left|\frac{C}{A}\right|^2, \tag{2.195}$$

with $J_C := J_R$. We have then

$$T + R = \frac{J_B + J_C}{J_A} = \frac{J_A}{J_A} = 1. \tag{2.196}$$

We consider now the case where $E < V_0$. For $x < 0$, we have the same solution as before. For $x > 0$ we can verify that changing $\bar{k} \to i\kappa$ we obtain the right solution given by

$$\psi(x) = Ce^{-i\kappa}. \tag{2.197}$$

Now,

$$\frac{B}{A} = \frac{k - i\kappa}{k + i\kappa} = -\left(\frac{\kappa + ik}{\kappa - ik}\right) = -e^{2i\delta(E)}, \tag{2.198}$$

where

$$\delta(E) = \arctan\left(\frac{k}{\kappa}\right) = \arctan\left(\sqrt{\frac{E}{V_0 - E}}\right). \tag{2.199}$$

Because the solution is real for $x > 0$ there is no probability current in that region, thus

$$J_C = 0, \tag{2.200}$$

and

$$J_A = J_B. \tag{2.201}$$

For $x < 0$ the solution is then

$$\begin{aligned}\psi(x) &= Ae^{ikx} - Ae^{2i\delta(E)}e^{-ikx} = Ae^{i\delta(E)}\left(e^{i(kx-\delta(E))} - e^{-i(kx-\delta(E))}\right) \\ &= 2iAe^{i\delta(E)}\sin(kx - \delta(E)),\end{aligned} \tag{2.202}$$

with

$$|\psi|^2 = 4|A|^2\sin^2(kx - \delta(E)). \tag{2.203}$$

We now consider wavepackets with $A = 1$ and $E > V_0$. The solution of Schrödinger's equation is

$$\Psi(x,t) = \begin{cases} \left(e^{ikx} + \frac{k-\bar{k}}{k+\bar{k}}e^{-ikx}\right)e^{-\frac{iEt}{\hbar}}, & x < 0 \\ \frac{2k}{k+\bar{k}}e^{i\bar{k}x}e^{-\frac{iEt}{\hbar}}, & x > 0. \end{cases} \tag{2.204}$$

By linearity, the following is still a solution

$$\Psi(x,t) = \begin{cases} \int_0^\infty \left[f(k)\left(e^{ikx} + \frac{k-\bar{k}}{k+\bar{k}}e^{-ikx}\right)e^{-\frac{iEt}{\hbar}}\right]dk, & x < 0, \\ \int_0^\infty \left[f(k)\frac{2k}{k+\bar{k}}e^{i\bar{k}x}e^{-\frac{iEt}{\hbar}}\right]dk, & x > 0, \end{cases} \tag{2.205}$$

where $k \in (0, \infty)$ to keep our directional interpretations of incoming/outgoing/reflected waves. We define the incident wavepacket

$$\Psi_{inc}(x < 0, t) = \int_0^\infty \left[f(k)e^{ikx}e^{-\frac{iEt}{\hbar}}\right]dk, \tag{2.206}$$

and the reflected wavepacket

$$\Psi_{ref}(x < 0, t) = \int_0^\infty \left[f(k)\left(\frac{k-\bar{k}}{k+\bar{k}}\right)e^{-ikx}e^{-\frac{iEt}{\hbar}}\right]dk, \tag{2.207}$$

and finally the transmitted wavepacket

$$\Psi_{trans}(x>0,t)=\int_0^\infty\left[f(k)\left(\frac{2k}{k+\bar{k}}\right)e^{i\bar{k}x}e^{-\frac{iEt}{\hbar}}\right]dk. \tag{2.208}$$

We consider from now on $f(k)$ to be real and localized at k_0, this allows one to use the stationary phase condition. For the incident wave, we have

$$\frac{d}{dk}\left(kx-\frac{Et}{\hbar}\right)\Big|_{k_0}=0, \tag{2.209}$$

and thus

$$x=\frac{\hbar k_0}{m}t, \tag{2.210}$$

using $E=\hbar^2k^2/(2m)$. The incident wave is coming from the left for time $t<0$. For the reflected wave, we have

$$\frac{d}{dk}\left(-kx-\frac{Et}{\hbar}\right)\Big|_{k_0}=0, \tag{2.211}$$

and thus

$$x=-\frac{\hbar k_0}{m}t. \tag{2.212}$$

The reflected wave is coming from the right for time $t>0$. For the transmitted wave we find

$$x=\frac{\hbar\bar{k}}{m}t, \tag{2.213}$$

which is satisfied for $t>0$.

The solution obtained in the case $E>V_0$ was given by

$$\Psi(x,t)=\begin{cases}e^{ikx}-e^{2i\delta(E)}e^{-ikx}, & x<0,\\ e^{-i\kappa}, & x>0,\end{cases} \tag{2.214}$$

and therefore

$$\Psi_{inc}(x<0,t)=\int_0^\infty\left[f(k)e^{ikx}e^{-\frac{iEt}{\hbar}}\right]dk, \tag{2.215}$$

and the reflected wavepacket

$$\Psi_{ref}(x<0,t)=-\int_0^\infty\left[f(k)e^{2i\delta(E)}e^{-ikx}e^{-\frac{iEt}{\hbar}}\right]dk. \tag{2.216}$$

The transmitted wavepacket in this case is not very interesting since it vanishes out. Considering again $f(k)$ to be real and localized at k_0, which allows one to use the stationary phase condition, for the incident wave we have the same result, while for the transmitted we obtain

$$\frac{d}{dk}\left(-kx+2\delta(E)-\frac{Et}{\hbar}\right)\Big|_{k_0}=0, \tag{2.217}$$

with

$$x=-\frac{\hbar k_0}{m}\left(t-2\hbar\delta'(E)\right). \tag{2.218}$$

In this case, there is a delay until the particle gets reflected back, which happens at $t=2\hbar\delta'(E)$ such that $x<0$. This delay can be used to find what type of potential we have for certain scatterings.

When $E < V_0$, can we find the particle in the forbidden region? If the particle is in the forbidden region, i.e. $x > 0$, then it should have negative kinetic energy since $E < V_0$. This seems somewhat contradictory. The forbidden region stretches to the order of $1/\kappa$ where $\kappa^2 = 2m(V_0 - E)/\hbar^2$. To find the particle in that region we would need to measure position with a precision $\Delta x \leq 1/\kappa$ and will have uncertainty in momentum which satisfies $\Delta p \geq \hbar/\Delta x \geq \hbar\kappa$. Now, the uncertainty in the kinetic energy is

$$KE = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2\kappa^2}{2m} = V_0 - E, \tag{2.219}$$

such that if a particle is indeed localized in the forbidden region the uncertainty in its momentum allows for a regular particle of zero momentum.

End of Lecture 16

2.12 Ramsauer–Townsend effect

Consider the potential

$$V(x) = \begin{cases} 0, & x < -a, \\ -V_0, & -a < x < a, \\ 0, & x > a, \end{cases} \tag{2.220}$$

where $V_0 > 0$ with $E > 0$. We know the solution is given by

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a, \\ Ce^{ik_2 x} + De^{-ik_2 x}, & -a < x < a, \\ Fe^{ikx}, & x > a, \end{cases} \tag{2.221}$$

where

$$\begin{cases} k^2 = \frac{2mE}{\hbar^2}, \\ k_2^2 = \frac{2m(E+V_0)}{\hbar^2}. \end{cases} \tag{2.222}$$

For $x < -a$ we have an incoming wave traveling to the right (with coefficient A, and a reflected part (with coefficient B). In the middle we have a transmitted (coefficient C) and reflected parts (coefficient D) and for $x > a$ we have only a transmitted part (coefficient F).

We can conjecture that the reflected coefficient R and transmission coefficient T satisfy

$$\begin{cases} R = \left|\frac{B}{A}\right|^2, \\ T = \left|\frac{F}{A}\right|^2, \end{cases} \tag{2.223}$$

such that from current conservation with $J_L \sim |A|^2 - |B|^2$ and $J_R \sim |F|^2$ we obtain $|A|^2 - |B|^2 = |F|^2$ and thus, dividing by $|A|^2$, we get $1 = R + T$.

To relate the coefficients in the wave function we consider the continuity of the wavefunction and its derivative which leads to

$$\frac{1}{T} = 1 + \frac{1}{4}\frac{V_0^2}{E(E+V_0)}\sin^2(2k_2 a). \tag{2.224}$$

Clearly $T \leq 1$ and we can see that as $E \to \infty$ we have $T \to 1$ and as $E \to 0$ we have $T \to 0$.
Rewriting the sin term in terms of an adimensional "energy" $e = E/V_0$, we have

$$2k_2 a = 2\sqrt{\frac{2ma^2(E+V_0)}{\hbar^2}} = 2\sqrt{\frac{2ma^2V_0(1+E/V_0)}{\hbar^2}} = 2Z_0\sqrt{1+e}, \tag{2.225}$$

where

$$Z_0 = \frac{2ma^2V_0}{\hbar^2}, \tag{2.226}$$

is considered the depth of the potential well. Then

$$\frac{1}{T} = 1 + \frac{1}{4e(1+e)}\sin^2(2Z_0\sqrt{1+e}). \tag{2.227}$$

For what values of the energy do we have perfect transmission, i.e $T = 1$? We compute

$$2Z_0\sqrt{1+e} = n\pi, \tag{2.228}$$

where $n \in \mathbb{N}$ satisfies $n \geq 2Z_0/\pi$, since $e > 0$. Thus, we have

$$4Z_0^2(1+e_n) = n^2\pi^2, \tag{2.229}$$

leading to

$$e_n = \frac{n^2\pi^2}{4Z_0^2} - 1, \tag{2.230}$$

and such that

$$E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} - V_0. \tag{2.231}$$

The resonance happens with for energies $\frac{n^2\pi^2\hbar^2}{2m(2a)^2}$ coincides with the energy levels of an infinite square well of width $2a$. Writing

$$k_2(2a) = \frac{2\pi}{\lambda}(2a) = n\pi, \tag{2.232}$$

we have

$$\frac{2a}{\frac{\lambda}{2}} = n. \tag{2.233}$$

This means that, when half the wavelength fits the width of the well an integer number of times, we have a resonance leading to total transmission.

Example: Consider $Z_0 = 13\pi/4$. We need $n \geq 13/2$, i.e. $n \geq 7, 8, 9, ...$ we have for example

$$e_7 = \frac{E_7}{V_0} = 0.15976, \tag{2.234}$$

and

$$e_8 = \frac{E_8}{V_0} = 0.514793, \tag{2.235}$$

and

$$e_9 = \frac{E_9}{V_0} = 0.91716. \tag{2.236}$$

The following figure shows a graph of the transmission $T(e)$.

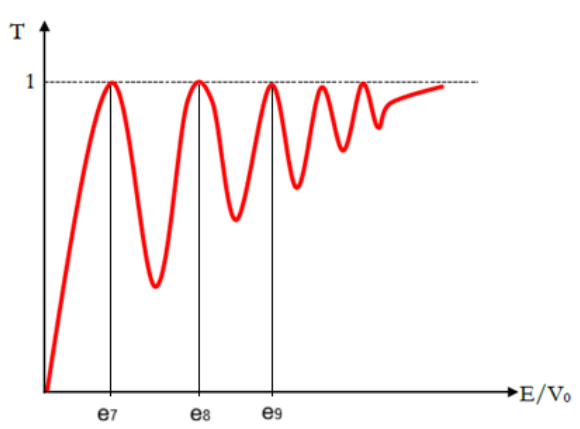

Figure 2: Transmission $T(e)$

In 1921, Ramsauer and Towsend scattered elastically low energy electrons off of rare gas atoms (with shells completely filled and thus highly non-reactive). The atom represents a spherical well that attracts the electrons (after entering the cloud) with the reflection coefficient representing a proxy for the scattering cross section.

2.13 Scattering in 1D

We now consider a potential

$$V(x) = \begin{cases} \infty, & x \leq 0, \\ V(x), & 0 < x < R, \\ 0, & x > R, \end{cases} \tag{2.237}$$

and suppose waves are coming from the right at infinity. We consider the following cases:

- $V(x) = 0$ in $0 < x < R$: The wavefunction is of the form

$$\phi(x) \sim e^{ikx} - e^{-ikx}, \tag{2.238}$$

since the boundary condition at $x = 0$ makes the ongoing and reflected coefficients be additive inverses. Multiplying by $1/(2i)$ we can write the solution as

$$\phi(x) = \frac{e^{ikx} - e^{-ikx}}{2i} = \sin(kx), \tag{2.239}$$

calling the outgoing wave

$$\phi_{\text{out}}(x) = \frac{e^{ikx}}{2i}, \tag{2.240}$$

and the incoming wave

$$\phi_{\text{inc}}(x) = -\frac{e^{-ikx}}{2i}. \tag{2.241}$$

- General $V(x)$ in $0 < x < R$: We take an incoming wave just like before

$$\psi_{\text{inc}}(x) = -\frac{e^{-ikx}}{2i}, \quad x > R, \tag{2.242}$$

while the outgoing wave is of the form

$$\psi_{\text{out}}(x) \sim \frac{e^{ikx}}{2i}, \tag{2.243}$$

but it cannot be the same. However, whatever is missing, can not be a function of x since it must be a solution of the Schrödinger's equation for $x > R$. Thus, we expect some constant multiple of the previous case. By current conservation we must have

$$|A|^2 = |B|^2, \tag{2.244}$$

such that $J_{\text{inc}} = J_{\text{ref}}$, and we conclude that the only possible factor is a phase shift. We write then

$$\psi_{\text{out}}(x) = \frac{e^{ikx}}{2i} e^{2i\delta(k)}. \tag{2.245}$$

The solution is then

$$\psi(x) = \frac{1}{2i}\left(e^{ikx+2i\delta} - e^{-ikx}\right) = \frac{e^{i\delta}}{2i}\left(e^{i(kx+\delta)-e^{-i(kx+\delta)}}\right) = e^{i\delta}\sin(kx+\delta), \;\; x > R. \tag{2.246}$$

We have then

$$|\phi(x)|^2 = \sin^2(kx), \tag{2.247}$$

and

$$|\psi(x)|^2 = \sin^2(kx+\delta). \tag{2.248}$$

Whatever feature of the wave occurs such that $kx = a_0$, i.e. $x = a_0/k$, in the latter case we have $k\tilde{x} + \delta = a_0$, or $\tilde{x} = a_0/k - \delta/k$. Thus, for $\delta > 0$, ψ is pulled in compared to ϕ, potential is attractive, while if $\delta < 0$, ψ is pushed out compared to ϕ, potential is repulsive.

We define the scattered wave ψ_s as the extra piece in the ψ solution that would vanish without the potential, which we write as

$$\psi := \phi + \psi_s. \tag{2.249}$$

Since the incoming waves are the same, ψ_s represents the difference in the outgoing waves. We have then

$$\psi_s = \psi - \phi = \frac{e^{ikx}}{2i}(e^{2i\delta} - 1) = e^{ikx}e^{i\delta}\left(\frac{e^{i\delta} - e^{-i\delta}}{2i}\right) = e^{ikx}e^{i\delta}\sin(\delta) =: A_s e^{ikx}, \tag{2.250}$$

where

$$A_s = e^{i\delta}\sin(\delta). \tag{2.251}$$

End of Lecture 17

We now consider the phenomena of time delay as we have seen for wave packets before. Let

$$\psi_{\text{inc}}(x,t) = \int_0^\infty f(k)e^{-ikx}e^{-iE(k)t/\hbar}dk, \tag{2.252}$$

which is valid for $x > R$ and

$$\psi_{\text{ref}}(x,t) = \int_0^\infty f(k)e^{ikx}e^{2i\delta(E)}e^{-iE(k)t/\hbar}dk, \tag{2.253}$$

valid again for $x > R$, where $f(k)$ is a function peaked at some value k_0.

Using the principle of stationary phase at $k = k_0$ we find for ψ_{inc}

$$x = -\frac{\hbar k_0 t}{m} =: v_g t, \tag{2.254}$$

where $t < 0$ and for ψ_{ref}

$$x = v_g(t - 2\hbar\delta'(E)), \tag{2.255}$$

which makes sense for $t > 2\hbar\delta'(E)$, showing there is a delayed in the reflected wavepacket, i.e.

$$\Delta t = 2\hbar\delta'(E) = 2\hbar\frac{d\delta}{dk}\frac{dk}{dE} = \frac{2}{\frac{1}{\hbar}\frac{dE}{dk}|_{k_0}}\frac{d\delta}{dk}\Big|_{k_0} = \frac{2}{v_g}\frac{d\delta}{dk}\Big|_{k_0}, \tag{2.256}$$

or dividing by R gives equivalently

$$\frac{1}{R}\frac{d\delta}{dk}\Big|_{k_0} = \frac{\Delta t}{\frac{2R}{v_g}}, \tag{2.257}$$

where the RHS corresponds to the delay divided by the free transit time.

Example: Let $E > 0$ and consider the potential

$$V(x) = \begin{cases} \infty, & x < 0, \\ -V_0, & 0 < x < a, \\ 0, & x > a. \end{cases} \tag{2.258}$$

The solution is given by

$$\psi(x) = \begin{cases} e^{i\delta}\sin(kx + \delta), & x > a \\ A\sin(k'x), & 0 < x < a, \end{cases} \tag{2.259}$$

where $k^2 = 2mE/\hbar^2$ and $k' = 2m(E + V_0)/\hbar^2$. From continuity of ψ at $x = a$, we get

$$A\sin(k'a) = e^{i\delta}\sin(ka + \delta), \tag{2.260}$$

while from the continuity of ψ' we get

$$Ak'\cos(k'a) = ke^{i\delta}\cos(ka + \delta). \tag{2.261}$$

Taking the ratio of these equations we get

$$\cot(ka + \delta) = \frac{k'}{k}\cot(k'a). \tag{2.262}$$

Using the trigonometric identity

$$\cot(A + B) = \frac{\cot(A)\cot(B) - 1}{\cot(A)\cot(B)} \tag{2.263}$$

we obtain

$$\frac{\cot(ka)\cot(\delta) - 1}{\cot(ka)\cot(\delta)} = \frac{k'}{k}\cot(k'a), \tag{2.264}$$

leading to

$$\cot(\delta) = \frac{\tan(ka) + \frac{k'}{k}\cot(k'a)}{1 - \frac{k'}{k}\cot(k'a)\tan(ka)}, \tag{2.265}$$

which gives us δ and therefore the meaningful quantity specifying the wavefunction. We now define the unit free variables

$$(ka)^2 = \frac{2mEa^2}{\hbar^2} =: u^2, \tag{2.266}$$

and

$$(k'a)^2 = \frac{2mEa^2}{\hbar^2} + \frac{2mV_0a^2}{\hbar^2} =: u^2 + z_0^2. \tag{2.267}$$

Using $k'a = \sqrt{z_0^2 + u^2}$ and $(k'a)/(ka) = \sqrt{1 + (z_0/u)^2}$ we can then write

$$\tan(\delta) = \frac{1 - \sqrt{1 + (z_0/u)^2}\cot(z_0^2 + u^2)\tan(u)}{\tan(u) + \sqrt{1 + (z_0/u)^2}\cot(z_0^2 + u^2)}, \tag{2.268}$$

which one can now plot using Mathematica for example. As $u \to 0$, $\tan(\delta) \to 0$ so $\delta(0) = 0$. **There's an intimate relation between how much the phase shifts and the number of bound states of the given potential**. This relation is called **Levinson's Theorem**.

2.14 Levinson's Theorem

Levinson's Theorem relates the number of bound states N of the potential to the excursion of the phase shift δ from $E = 0$ to $E = \infty$. In particular

$$N = \frac{1}{\pi}(\delta(0) - \delta(\infty)). \tag{2.269}$$

We consider a potential of the form

$$V(x) = \begin{cases} \infty, & x \leq 0, \\ V(x), & 0 < x < R, \\ 0, & R < x < L, \infty, \quad x > L, \end{cases} \tag{2.270}$$

where $L >> R$ is a regulator to avoid a continuum of states. We start again in the case where $V \equiv 0$ in $0 < x < R$ with $E > 0$. The solutions where $\phi(x) = \sin(kx)$ but now we also require that $\phi(L) = 0$. Thus, we have

$$kL = n\pi, \quad n \in \mathbb{N}. \tag{2.271}$$

In a range dk, we have

$$dkL = dn\pi, \tag{2.272}$$

where dn is the number of states in the range dk, such that

$$dn = \frac{L}{\pi}dk. \tag{2.273}$$

We now do the same for $V \neq 0$, for $x > R$ we have

$$\psi(x) = e^{i\delta}\sin(kx + \delta(k)), \tag{2.274}$$

and again we must have $\psi(L) = 0$. This leads to

$$kL + \delta(k) = m\pi, \quad m \in \mathbb{N}, \tag{2.275}$$

and thus

$$dkL + \frac{d\delta}{dk}dk = dm\pi, \tag{2.276}$$

leading to

$$dm = \frac{L}{\pi}dk + \frac{1}{\pi}\frac{d\delta}{dk}dk, \tag{2.277}$$

the number of positive energy states in dk for $V \neq 0$.

The number of positive energy bound states lost in the interval dk as the potential turns on, i.e. goes from $V = 0$ to some $V \neq 0$, is

$$dn - dm = -\frac{1}{\pi}\frac{d\delta}{dk}dk. \tag{2.278}$$

Thus, the total numbers of lost states is given by

$$\int_0^\infty -\frac{1}{\pi}\frac{d\delta}{dk}dk = \frac{1}{\pi}(\delta(0) - \delta(\infty)) = N_{\text{bound states}}, \tag{2.279}$$

since we assume there are no lost states in total.

Remark 2.6. *The differentials with respect to a non-continuous variable n are quite sketchy. The argument is not rigorous at all.*

End of Lecture 18

3 1D Scattering, Angular Momentum and Central Potentials

References

[GS18] David J. Griffiths and Darrell F. Schroeter. *Introduction to quantum mechanics*. Third edition. Cambridge ; New York, NY: Cambridge University Press, 2018. ISBN: 978-1-107-18963-8.