Quantum Mechanics I

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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. The main textbook used is [GS18].

Contents

1 Basic Concepts **2**

1.1 Linearity . . . 2
1.2 Complex Numbers . . . 2
1.3 Determinism . . . 2
1.4 Nature of Superposition in Quantum Mechanics . . . 3
1.5 The photoelectric effect . . . 4
1.6 Compton Scattering . . . 4
1.7 de Broglie wave/particle duality . . . 5
1.8 Deriving Matter Waves (Wave Function) . . . 5
1.9 Schrödinger's Equation . . . 7
1.10 Interpreting the Wave Function . . . 9
1.11 Normalizable Wave Functions . . . 9
1.12 Wave Packets and Fourier Representation . . . 12
1.13 Time Evolution of a Free Particle . . . 15
1.14 Momentum Space . . . 15
1.15 Expectation Values of Operators . . . 17
1.16 Observables and Hermitian Operators . . . 19

2 Quantum Physics in 1D Potentials **24**

2.1 Stationary Sates . . . 24

3 1D Scattering, Angular Momentum and Central Potentials **25**

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.

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

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

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

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

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 of $\omega(k)$ 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

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

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

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

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

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

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.

- Step 3: At a later time t we just evaluate (CLAIM)

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \Phi(k) e^{i(kx - \omega(k)t)} dk, \tag{1.106}$$

  where $\hbar\omega(k) = E = p^2/(2m) = \hbar^2 k^2/(2m)$. To check the claim, we just need to check that $\Psi(x, t)$ verifies the Schrödinger's equation with initial condition $\Psi(x, 0)$ at $t = 0$. This is clear.

- 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

$$\begin{aligned} \Psi(x) &= \frac{1}{2\pi} \int_{\mathbb{R}} \left(\int_{\mathbb{R}} \Psi(x') e^{-ikx'} dx' \right) e^{ikx} dk \\ &= \int_{\mathbb{R}} \Psi(x') \left(\frac{1}{2\pi} \int_{\mathbb{R}} e^{ik(x-x')} dk \right) dx', \end{aligned} \tag{1.107}$$

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

Remark 1.9. *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)

$$\delta(x'-x) := \frac{1}{2\pi}\int_{\mathbb{R}} e^{ik(x'-x)}dk, \tag{1.108}$$

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

$$\begin{aligned}\int_{\mathbb{R}} |\Psi(x)|^2 dx &= \int_{\mathbb{R}} \Psi^*(x)\Psi(x)dx \\ &= \int_{\mathbb{R}} \left[\left(\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \Phi^*(k)e^{-ikx}dk\right)\left(\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \Phi(k')e^{ik'x}dk'\right)\right]dx.\end{aligned} \tag{1.109}$$

Let us define

$$f(x) := \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \Phi^*(k)e^{-ikx}dk, \tag{1.110}$$

$$g(x) := \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \Phi(k')e^{ik'x}dk', \tag{1.111}$$

and

$$\tilde{f}(k) := \frac{1}{\sqrt{2\pi}}\Phi^*(k)e^{-ikx}. \tag{1.112}$$

$$\tilde{g}(k') := \frac{1}{\sqrt{2\pi}}\Phi(k')e^{ik'x}. \tag{1.113}$$

By Fubini's Theorem, the above integral is then

$$\begin{aligned}\int_{\mathbb{R}}\left[\int_{\mathbb{R}}\left(g(x)\tilde{f}(k)\right)dk\right]dx &= \int_{\mathbb{R}}\left[\int_{\mathbb{R}}\left(g(x)\tilde{f}(k)\right)dx\right]dk \\ &= \int_{\mathbb{R}}\left[\int_{\mathbb{R}}\left(\left(\int_{\mathbb{R}}\tilde{g}(k')dk'\right)\tilde{f}(k)\right)dx\right]dk \\ &= \int_{\mathbb{R}}\left[\int_{\mathbb{R}}\left(\left(\int_{\mathbb{R}}\tilde{g}(k')\tilde{f}(k)\right)dx\right)dk'\right]dk \\ &= \int_{\mathbb{R}}\left[\Phi^*(k)\int_{\mathbb{R}}\left[\Phi(k')\underbrace{\left(\int_{\mathbb{R}}\left(\frac{1}{2\pi}e^{-ix(k'-k)}\right)dx\right)}_{\delta(k'-k)}\right]dk'\right]dk \\ &= \int_{\mathbb{R}}\left[\Phi^*(k)\Phi(k)\right]dk = \int_{\mathbb{R}}|\Phi(k)|^2dk.\end{aligned} \tag{1.114}$$

This is called Parseval's Theorem. Thus, if

$$\int_{\mathbb{R}}|\Psi(x)|^2dx = 1, \tag{1.115}$$

we have

$$\int_{\mathbb{R}}|\Phi(k)|^2dk = 1, \tag{1.116}$$

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

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Phi(k) e^{ipx\hbar} dk, \tag{1.117}$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Psi(x) e^{-ipx\hbar} dx. \tag{1.118}$$

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

$$\int_{\mathbb{R}} |\Psi(x)|^2 dx = \int_{\mathbb{R}} |\Phi(p)|^2 dp = 1. \tag{1.119}$$

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

$$\Psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \Phi(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} d^3p. \tag{1.120}$$

$$\Psi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \Psi(\vec{x}) e^{-i\vec{p}\cdot\vec{x}/\hbar} d^3x. \tag{1.121}$$

$$\delta^3(\vec{x'} - \vec{x}) := \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{i\vec{k}\cdot(\vec{x'}-\vec{x})} dk, \tag{1.122}$$

and

$$\int_{\mathbb{R}^3} |\Psi(\vec{x})|^2 d^3x = \int_{\mathbb{R}^3} |\Phi(\vec{p})|^2 d^3p = 1. \tag{1.123}$$

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 $\{p_1, p - 2, ..., p_n\}$.

$$\mathbb{E}(Q) = \langle Q \rangle := \sum_{i=1}^{n} q_i p_i. \tag{1.124}$$

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

$$\mathbb{E}(Q) = \langle Q \rangle := \int_{\mathbb{R}} q p(Q = q) dq. \tag{1.125}$$

Recalling that

$$\Psi^*(x,t)\Psi(x,t)dx) = |\Psi(x,t)|^2, \tag{1.126}$$

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

$$\langle \hat{x} \rangle(t) := \int_{\mathbb{R}} x |\Psi(x,t)|^2 dx. \tag{1.127}$$

Similarly, as said above,

$$\Phi^*(p,t)\Phi(p,t)dp = |\Phi(p,t)|^2, \tag{1.128}$$

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

$$\langle \hat{p} \rangle(t) := \int_{\mathbb{R}} p \Phi^*(p,t)\Phi(p,t) dp. \tag{1.129}$$

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

$$\begin{aligned}\langle \hat{p} \rangle(t) &:= \int_{\mathbb{R}} \left[p \left(\frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Psi^*(x',t) e^{ipx'/\hbar} dx' \right) \left(\frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Psi(x,t) e^{-ipx/\hbar} dx \right) \right] dp \\ &= \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left[\Psi^*(x',t) \int_{\mathbb{R}} \left(\Psi(x,t) \int_{\mathbb{R}} p e^{ip(x'-x)/\hbar} dp \right) dx \right] dx'.\end{aligned} \tag{1.130}$$

We now look at the term

$$\int_{\mathbb{R}} p e^{ip(x'-x)/\hbar} dp, \tag{1.131}$$

which we can write as

$$i\hbar \int_{\mathbb{R}} \frac{\partial}{\partial x} \left(e^{ip(x'-x)/\hbar} \right) dp. \tag{1.132}$$

Therefore,

$$\begin{aligned}\langle \hat{p} \rangle(t) &= \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left[\Psi^*(x',t) \int_{\mathbb{R}} \left(\Psi(x,t) i\hbar \int_{\mathbb{R}} \frac{\partial}{\partial x} \left(e^{ip(x'-x)/\hbar} \right) dp \right) dx \right] dx' \\ &= \int_{\mathbb{R}} \left[\Psi^*(x',t) \int_{\mathbb{R}} \left(\Psi(x,t) i\hbar \frac{\partial}{\partial x} \underbrace{\left[\frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right]}_{\delta(x'-x)} \right) dx \right] dx'.\end{aligned} \tag{1.133}$$

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

$$\begin{aligned}&\int_{\mathbb{R}} \Psi^*(x',t) \Bigg(\left[\frac{i}{2\pi} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right] \Psi(x,t) \Bigg|_{x=-\infty}^{x=\infty} \\ &\qquad - \int_{\mathbb{R}} \left(i\hbar \frac{\partial \Psi(x,t)}{\partial x} \right) \left[\frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right] dx \Bigg) dx'\end{aligned} \tag{1.134}$$

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

$$\begin{aligned}&- \int_{\mathbb{R}} \Psi^*(x',t) \int_{\mathbb{R}} \left(i\hbar \frac{\partial \Psi(x,t)}{\partial x} \right) \left[\frac{1}{2\pi\hbar} \int_{\mathbb{R}} \left(e^{ip(x'-x)/\hbar} \right) dp \right] dx dx' \\ = \;& \frac{\hbar}{i} \int_{\mathbb{R}} \Psi^*(x',t) \int_{\mathbb{R}} \left(\frac{\partial \Psi(x,t)}{\partial x} \right) \delta(x-x') dx dx' \\ = \;& \int_{\mathbb{R}} \left[\frac{\hbar}{i} \frac{\partial \Psi}{\partial x}(x,t) \left(\int_{\mathbb{R}} \left(\Psi^*(x',t) \delta(x-x') \right) dx' \right) \right] dx \\ = \;& \int_{\mathbb{R}} \left[\frac{\hbar}{i} \frac{\partial \Psi}{\partial x}(x,t) \Psi^*(x,t) \right] dx.\end{aligned} \tag{1.135}$$

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

$$\langle \hat{p} \rangle(t) = \int_{\mathbb{R}} \left[\Psi^*(x,t) \frac{\hbar}{i} \frac{\partial \Psi}{\partial x}(x,t) \right] dx, \tag{1.136}$$

where

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}. \tag{1.137}$$

In general we define

$$\langle \hat{Q} \rangle(t) = \int_{\mathbb{R}} \Psi^*(x,t) \hat{Q} \Psi(x,t) dx. \tag{1.138}$$

Remark 1.10. *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

$$\hat{T} = \frac{\hat{p}^2}{2m}. \tag{1.139}$$

In momentum space, we simply have

$$\langle \hat{T} \rangle(t) = \int_{\mathbb{R}} \Phi^*(p,t) \frac{p^2}{2m} \Phi(p,t) dp. \tag{1.140}$$

In position space, we have

$$\begin{aligned} \langle \hat{T} \rangle(t) &= \int_{\mathbb{R}} \Psi^*(x,t) \frac{i}{\hbar} \frac{\partial}{\partial x} \left(\frac{i}{\hbar} \frac{\partial}{\partial x} \Psi(x,t) \right) dp \\ &= -\frac{\hbar^2}{2m} \int_{\mathbb{R}} \Psi^*(x,t) \frac{\partial^2 \Psi}{\partial x^2}(x,t) dx \\ &= \frac{\hbar^2}{2m} \int_{\mathbb{R}} \frac{\partial \Psi^*}{\partial x}(x,t) \frac{\partial \Psi}{\partial x}(x,t) dx = \frac{\hbar^2}{2m} \int_{\mathbb{R}} |\Psi(x,t)|^2 dx, \end{aligned} \tag{1.141}$$

using integration by parts.

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

$$\begin{aligned} \frac{d}{dt} \langle \hat{Q} \rangle(t) &= \frac{d}{dt} \int_{\mathbb{R}} \Psi^*(x,t) \hat{Q} \Psi(x,t) dx. \\ &= \int_{\mathbb{R}} \left(\frac{\partial \Psi^*}{\partial t}(x,t) \hat{Q} \Psi(x,t) + \Psi^*(x,t) \hat{Q} \frac{\partial \Psi}{\partial t}(x,t) \right) dx. \end{aligned} \tag{1.142}$$

Using Schrödinger's equation we obtain

$$\begin{aligned} &\int_{\mathbb{R}} \left(\frac{\partial \Psi^*}{\partial t}(x,t) \hat{Q} \Psi(x,t) + \Psi^*(x,t) \hat{Q} \frac{\partial \Psi}{\partial t}(x,t) \right) dx \\ = &\int_{\mathbb{R}} \left(\frac{i}{\hbar} (\hat{H}\Psi)^* \hat{Q} \Psi - \Psi^* \frac{i}{\hbar} (\hat{Q}\hat{H}\Psi) \right) dx. \end{aligned} \tag{1.143}$$

Looking at

$$\begin{aligned} i\hbar \frac{d}{dt} \langle \hat{Q} \rangle(t) &= \int_{\mathbb{R}} \left(\Psi^*(\hat{Q}\hat{H}\Psi) - (\hat{H}\Psi)^* \hat{Q} \Psi \right) dx \\ &= \int_{\mathbb{R}} \left(\Psi^*(\hat{Q}\hat{H}\Psi) - \Psi^* \hat{H} \hat{Q} \Psi \right) dx \\ &= \int_{\mathbb{R}} \Psi^*(x,t) [\hat{Q}, \hat{H}] \Psi(x,t) dx. \end{aligned} \tag{1.144}$$

So we found out that

$$i\hbar \frac{d}{dt} \langle \hat{Q} \rangle(t) = \langle [\hat{Q}, \hat{H}] \rangle(t). \tag{1.145}$$

Remark 1.11. *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

$$(\Psi, \hat{Q}\Phi) := \int_{\mathbb{R}} \Psi^* \hat{Q}\Phi dx = \int_{\mathbb{R}} (\hat{Q}\Psi)^* \Phi dx =: (\hat{Q}\Psi, \Phi). \tag{1.146}$$

for any wavefunctions Ψ and Φ.

In this notation, the expectation value of Q becomes

$$\langle \hat{Q} \rangle_\Psi = \int_{\mathbb{R}} \Psi^* \hat{Q}\Psi dx = (\Psi, \hat{Q}\Psi). \tag{1.147}$$

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

$$\begin{aligned} (\langle \hat{Q} \rangle_\Psi)^* = (\Psi, \hat{Q}\Psi)^* &= \left(\int_{\mathbb{R}} \Psi^* \hat{Q}\Psi dx \right)^* \\ &= \int_{\mathbb{R}} \left(\Psi^* \hat{Q}\Psi \right)^* dx = \int_{\mathbb{R}} \Psi (\hat{Q}\Psi)^* dx \\ &= \int_{\mathbb{R}} (\hat{Q}\Psi)^* \Psi dx = (\hat{Q}\Psi, \Psi) = (\Psi, \hat{Q}\Psi) = \langle \hat{Q} \rangle_\Psi . \end{aligned} \tag{1.148}$$

■

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

$$\hat{Q}\Psi_i = \lambda_i \Psi_i, \tag{1.149}$$

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

Proof. We have

$$\langle \hat{Q} \rangle_{\Psi_i} = (\Psi_i, \hat{Q}\Psi_i) = (\Psi_i, \lambda_i \Psi_i) = \lambda_i (\Psi_i, \Psi_i) = \lambda_i, \tag{1.150}$$

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.*

$$\begin{aligned} \hat{Q}\Psi_1 &= q_1 \Psi_1 \\ \hat{Q}\Psi_2 &= q_2 \Psi_2 \\ &\vdots \end{aligned} \tag{1.151}$$

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

$$(\Psi_i, \Psi_j) = \int_{\mathbb{R}} \Psi_i^* \Psi_j dx = \delta_{ij}. \tag{1.152}$$

Proof. Consider

$$(\Psi_i, \hat{Q}\Psi_j) = q_j(\Psi_i, \Psi_j). \tag{1.153}$$

$$(\hat{Q}\Psi_i, \Psi_j) = q_i(\Psi_i, \Psi_j). \tag{1.154}$$

Then, since these are the same, we have

$$(q_i - q_j)(\Psi_i, \Psi_j) = 0, \tag{1.155}$$

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

Remark 1.12. *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.*

$$\Psi(x) = \sum_i \alpha_i \Psi_i, \tag{1.156}$$

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.

$$\begin{aligned}(\Psi_i, \Psi) &= \int_{\mathbb{R}} \Psi_i^* \Psi dx = \int_{\mathbb{R}} \Psi_i^* \left(\sum_j \alpha_j \Psi_j\right) dx \\ &= \int_{\mathbb{R}} \left(\sum_j \alpha_j \Psi_i^* \Psi_j\right) dx = \sum_j \alpha_j \int_{\mathbb{R}} \Psi_i^* \Psi_j dx \\ &= \alpha_j \delta_{ij} = \alpha_i.\end{aligned} \tag{1.157}$$

Remark 1.13. *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

$$1 = \int_{\mathbb{R}} |\Psi|^2 dx = \int_{\mathbb{R}} \left(\sum_i \alpha_i \Psi_i\right)^* \left(\sum_j \alpha_j \Psi_j\right) dx = \sum_i \sum_j \alpha^i \alpha_j \int_{\mathbb{R}} \Psi_i^* \Psi_j dx = \sum_i |\alpha_i|^2. \tag{1.158}$$

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

$$p_i = |\alpha_i|^2 = |(\Psi_i, \Psi)|^2. \tag{1.159}$$

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

$$\begin{aligned}\langle\hat{Q}\rangle_\Psi = (\Psi,\hat{Q}\Psi) = \left(\sum_i \alpha_i\Psi_i, \hat{Q}(\sum_j \alpha_j\Psi_j)\right) &= \sum_i\sum_j \alpha_i^*\alpha_j(\Psi_i, q_j\Psi_j) \\ = \sum_i\sum_j \alpha_i^*\alpha_j q_j\delta_{ij} = \sum_i |\alpha_i|^2 q_i.\end{aligned} \tag{1.160}$$

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

Example (particle in a circle): Consider a line $[0,L]$ and identify its two endpoints, i.e. $0\leftrightarrow L$. This is topologically just S^1, although not necessarily the circle. Consider the wavefunction on S^1 given by

$$\Psi(x,t=0) = \sqrt{\frac{2}{L}}\left(\frac{1}{\sqrt{3}}\sin\left(\frac{2\pi x}{L}\right) + \sqrt{\frac{2}{3}}\cos\left(\frac{6\pi x}{L}\right)\right). \tag{1.161}$$

Clearly $\Psi(0)=\Psi(L)$. If we measure momentum, what are the possible values and their corresponding probabilities?

We guess the momentum wavefunction

$$... \tag{1.162}$$

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

$$\mathbb{E}\left((\Delta Q)^2\right) = \sum_i (q_i - \mathbb{E}(Q))^2 \geq 0. \tag{1.163}$$

Recalling that, for any random variable X we have

$$\mathbb{E}\left[(X-\bar{X})^2\right] = \mathbb{E}[X^2] - (\mathbb{E}[X])^2. \tag{1.164}$$

Then, for Q we have

$$\mathbb{E}\left((\Delta Q)^2\right) = \mathbb{E}[Q^2] - (\mathbb{E}[Q])^2 \geq 0, \tag{1.165}$$

or equivalently

$$\mathbb{E}[Q^2] \geq (\mathbb{E}[Q])^2. \tag{1.166}$$

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

$$\mathbb{E}\left[(\Delta\hat{Q})^2\right]_\Psi = \mathbb{E}[\hat{Q}^2]_\Psi - (\mathbb{E}[\hat{Q}])^2_\Psi := \langle\hat{Q}^2\rangle - \langle\hat{Q}\rangle^2. \tag{1.167}$$

Proposition 1.6. *We have*

$$\langle(\Delta\hat{Q})^2\rangle_\Psi = \langle(\hat{Q}-\langle\hat{Q}\rangle)^2\rangle \tag{1.168}$$

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*

$$\langle(\Delta\hat{Q})^2\rangle_\Psi = \int_{\mathbb{R}} \left|(\hat{Q}-\langle\hat{Q}\rangle)\Psi\right|^2 dx \tag{1.169}$$

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

$$\begin{aligned} \langle (\Delta \hat{Q})^2 \rangle_\Psi &= \int_{\mathbb{R}} \Psi^* (\hat{Q} - \mathbb{E}(\hat{Q})((\hat{Q} - \mathbb{E}(\hat{Q}))\Psi)) = \int_{\mathbb{R}} (\hat{Q} - \mathbb{E}(\hat{Q})\Psi)^* ((\hat{Q} - \mathbb{E}(\hat{Q}))\Psi)) \\ &= \int_{\mathbb{R}} \left| (\hat{Q} - \langle \hat{Q} \rangle)\Psi \right|^2 dx. \end{aligned} \tag{1.170}$$

■

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

$$\langle \hat{Q} \rangle_\Psi = \lambda \int_{\mathbb{R}} \Psi^* \Psi dx = \lambda, \tag{1.171}$$

and thus

$$\hat{Q}\Psi = \langle \hat{Q} \rangle_\Psi \Psi. \tag{1.172}$$

Furthermore

$$\langle (\Delta \hat{Q})^2 \rangle_\Psi = \int_{\mathbb{R}} \left| (\hat{Q} - \langle \hat{Q} \rangle)\Psi \right|^2 dx = \int_{\mathbb{R}} |\lambda\Psi - \lambda\Psi|^2 = 0. \tag{1.173}$$

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

End of Lecture 9

2 Quantum Physics in 1D Potentials

2.1 Stationary Sates

⟨IN PROGRESS⟩

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.