

# FYS2140 Guide - Quantum Physics

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# Introduction

This booklet contains a summary of all the lecture notes from our FYS2140 - Quantum Physics course. At the beginning of each lecture, our professor would quickly repeat the most important details from the previous lecture; these notes are the source of the material in this pamphlet, and is intended as a quick reference in case the reader has (for example) forgotten a detail about an equation.

## 1 Statistics

In Quantum Mechanics, the laws of motion are governed by statistics; there are a multitude of values that we can never calculate with 100% certainty. Fortunately, we can still find the probability of such values by using basic statistical concepts.

### 1.1 Expected Values

The probability of finding a continuously distributed value in the range of  $[x, x + dx]$  is given by the products of the probability density function  $\rho(x)$  and the infinitesimal change  $dx$ .

$$\langle x \rangle = \int_{-\infty}^{\infty} x \rho(x) dx \quad (1)$$

Using the product  $\rho(x)dx$ , we can find the *expected value*<sup>1</sup> (or *expectation value*) of a given  $x$  via (1). This is a rather basic example however, as it is possible to find the expectation value for many different things.

### 1.2 Variance

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \quad (2)$$

In many cases, it is necessary to find the *variance*<sup>2</sup>  $\sigma_x$  of an expectation value  $\langle x \rangle$  to be able to determine things such as standard deviation. To accomplish this, we can use (2).

## 2 Waves

$$\frac{\partial^2}{\partial t^2} \xi(x, t) = [c^2 \nabla^2 + V(x)] \xi \quad (3)$$

A particle can be described as a *complex wavefunction*  $\Psi$  (or for EM-waves  $\xi$ ), which is itself a solution of a given *wave equation* [for example, the general EM-wave equation is shown in (3)]; the wavefunction we use to describe non-relativistic particles is called **Schrödinger's Equation**.

$$A(x, t) = A_0 \cos(kx - \omega t + \varphi) \quad (4)$$

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<sup>1</sup>[https://en.wikipedia.org/wiki/Expected\\_value#Absolutely\\_continuous\\_case](https://en.wikipedia.org/wiki/Expected_value#Absolutely_continuous_case)

<sup>2</sup><https://en.wikipedia.org/wiki/Variance#Definition>

A localized particle can be described as the sum of a set of planewaves<sup>3</sup> with different  $k$  values  $k = \frac{2\pi}{\lambda}$ , known as a *wavepacket*<sup>4</sup>; (4) is the generalized form of a plane wave.

## 2.1 The Dispersion Relation

$$\omega(k) = \frac{\hbar k^2}{2m} \quad (5)$$

The *De Broglie* dispersion relation<sup>5</sup> [shown in (5)] is a useful value from which we can determine the *phase velocity*  $v_f$  and *group velocity*  $v_g$ .

$$v_f = \frac{\omega}{k} \quad (6)$$

The **Phase Velocity** is essentially the velocity of our wave, and is shown in (6).

$$v_g = \frac{d\omega}{dk} \quad (7)$$

The **Group Velocity** is the particle's velocity, and is shown in (7).

**Step-by-step** If we wish to find our phase velocity or group velocity, we can follow the steps below to easily set up our equations (6) and (7):

1. Find  $E(p)$
2. Replace  $E$  with  $\hbar\omega$
3. Replace  $p$  with  $\hbar k$
4. Solve for  $\omega(k)$

## 3 Bra-ket Notation

When dealing with the wavefunction  $\Psi$ , it is possible to express certain concepts via the usage of *bras* and *kets* for a more elegant way of representing values.

$$\langle \Psi_i | \Psi_j \rangle = \int_{-\infty}^{\infty} \Psi_i^* \Psi_j dx \quad (8)$$

A complete bra-ket<sup>6</sup> as seen on the left-hand side of (8), and is defined by the right-hand side. Within this bra-ket, the *bra* is represented by  $\langle \Psi_i |$ , while the *ket* is represented as  $|\Psi_j\rangle$ .

<sup>3</sup>[https://en.wikipedia.org/wiki/Plane\\_wave#Mathematical\\_representations](https://en.wikipedia.org/wiki/Plane_wave#Mathematical_representations)

<sup>4</sup>[https://en.wikipedia.org/wiki/Wave\\_packet#Gaussian\\_wave\\_packets\\_in\\_quantum\\_mechanics](https://en.wikipedia.org/wiki/Wave_packet#Gaussian_wave_packets_in_quantum_mechanics)

<sup>5</sup>[https://en.wikipedia.org/wiki/Dispersion\\_relation#De\\_Broglie\\_dispersion\\_relations](https://en.wikipedia.org/wiki/Dispersion_relation#De_Broglie_dispersion_relations)

<sup>6</sup>[https://en.wikipedia.org/wiki/Bra%E2%80%93ket\\_notation](https://en.wikipedia.org/wiki/Bra%E2%80%93ket_notation)

## 4 Schrödinger's Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[ \frac{-\hbar^2}{2m} \nabla^2 + V(x) \right] \Psi \quad (9)$$

Schrödinger's equation<sup>7</sup> is the wave equation that is used to describe the movement of particles in terms of a wavefunction  $\Psi(x, t)$  – it is shown in its general form in (9). We can do many things with this equation and wavefunction, but this will be described later in detail.

### 4.1 Superposition of Waves

$$A(x, t) = A_0(k) e^{i(kx - \omega t)} \quad (10)$$

Since our wavefunction  $\Psi(x, t)$  is a *wavepacket* (as discussed previously in Section 2), it consists of many waves of the form shown in (10).

$$\Psi(x, t) = \int_{-\infty}^{\infty} A_0(k) e^{i(kx - \omega t)} dk \quad (11)$$

If we want to construct our wavefunction, we can sum over all our waves for varying values of the wavenumber  $k$ , as seen in (11).

### 4.2 The Probabilistic Interpretation of Matter Waves

Using the knowledge we gained in Section 1, we can deduce that our wavefunction  $\Psi(x, t)$  can actually be used as part of a probabilistic density function – one which can be used to determine all matter of properties, such as position, momentum, and energy (among others.)

$$P_{a,b}(t) = \int_a^b |\Psi(x, t)|^2 dx \quad (12)$$

We see in (12) that we can use the square of the absolute value of  $\Psi$  as our probabilistic density function.

$$\rho(x) = |\Psi(x, t)|^2 = \Psi^* \Psi \quad (13)$$

Since  $\Psi$  is usually complex, we can find our probability density function in two ways, as shown in (13).

$$\rho(x) = \langle \Psi | \Psi \rangle \quad (14)$$

If we wish to represent this probability density using bra-ket notation, we can use (14).

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<sup>7</sup>[https://en.wikipedia.org/wiki/Schr%C3%B6dinger\\_equation](https://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation)

### 4.3 Normalization

Due to the nature of statistics, it is the case that there is impossible for a probability to ever be greater than 100% – in the case of physics, we often tend to drop the percentage sign and use the number 1 as our 100%. Since this is the case, we should take care to make sure the integral of the probability density function  $\Psi^*\Psi$  over infinity is always equal to one.

$$\langle\Psi|\Psi\rangle = \int_{-\infty}^{\infty} \Psi^*\Psi dx = 1 \quad (15)$$

To successfully normalize<sup>8</sup> a wavefunction, we must begin by solving the equation shown in (15); once this has been integrated, there will most likely be a constant (let's call it  $A$ , and assume it is contained within  $\Psi$  from the start) on the left-hand side of the equation. The final step then is to solve for  $A$  and replace the  $A$  in  $\Psi(x, t)$  with the new, normalized coefficient.

Two important things to bear in mind:

- Normalization is *independent* of time
- Normalization requires that  $|\Psi| \rightarrow 0$  as  $|x| \rightarrow \infty$

## 5 Expectation Values

As mentioned in Section 1.1: Expected Values, we can integrate over a probability density equation to give us useful information about a variety of things. In quantum mechanics, we can for example use our wavefunction  $\Psi$  as a way to determine "position" and "momentum" (these are in quotes due to the fact that we can never know their *exact* values) by using **operators**.

### 5.1 Operators

In general, we will from now on be using position and momentum as the basis for all other equations (when it is possible). For example, we will represent kinetic energy not as  $E_K = \frac{1}{2}mv^2$ , but rather as  $E_K = \frac{p^2}{2m}$ . This is helpful due to the fact that it allows us to simplify the way we calculate our expectation values.

To understand how we will use position and movement as our **operators**<sup>9</sup>, we must first define them.

#### Definition

$$\hat{x} = x \quad (16)$$

The operator for position  $\hat{x}$  is shown in (16).

$$\hat{p} = \frac{\hbar}{i} \nabla x \quad (17)$$

The operator for momentum  $\hat{p}$  is shown in (17).

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<sup>8</sup>[https://en.wikipedia.org/wiki/Wave\\_function#Position-space\\_wave\\_functions](https://en.wikipedia.org/wiki/Wave_function#Position-space_wave_functions)

<sup>9</sup>[https://en.wikipedia.org/wiki/Operator\\_\(physics\)#Operators\\_in\\_quantum\\_mechanics](https://en.wikipedia.org/wiki/Operator_(physics)#Operators_in_quantum_mechanics)

## 5.2 Operators Applied

$$\langle Q(\hat{x}, \hat{p}) \rangle = \int_{-\infty}^{\infty} \Psi^* Q\left(x, \frac{\hbar}{i} \nabla\right) \Psi dx \quad (18)$$

Let us now use our operators to find our expectation values. First of all, let us set up a general function  $Q$  of position and momentum; if we wish to determine the expectation value of  $Q$ , we can plug it into (18). Although this may seem to be a bit convoluted, in practice it could not be simpler – this is better understood via example.

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi dx \quad (19)$$

If we take the expectation value of  $x$  as an example, we can see from (19) that all we need to do is plug  $x$  in between our conjugates to find our result.

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \frac{\hbar}{i} \nabla \Psi dx \quad (20)$$

To find the expectation value of  $p$ , we can simply plug the operator for momentum in between our conjugates, as seen in (20).

$$\langle x \rangle = \langle \Psi | x | \Psi \rangle \quad (21)$$

$$\langle p \rangle = \left\langle \Psi \left| \frac{\hbar}{i} \nabla \right| \Psi \right\rangle \quad (22)$$

If we wish to instead use bra-ket notation, we can simply take our operator and place it in the left side of the ket, as seen in (21) and (22).

## 5.3 Ehrenfest's Theorem for Momentum

In general, we know that momentum is the product of mass and velocity. In addition to this, we know that velocity is the first time derivative of position.

$$\langle p \rangle = m \langle v \rangle = m \nabla \langle x \rangle \quad (23)$$

We can use this relation to simplify finding the expectation value of momentum<sup>10</sup> in some cases via (23). An example of this being useful is in the case where  $\langle x \rangle = \text{constant}$ , since taking its derivative would give us zero and prevent us from needing to calculate another integral.

## 5.4 Hermitian Operators

Let us begin with a postulate:

For all **observable**  $A$ , there exists a **Hermitian operator**  $\hat{A}$ .

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<sup>10</sup>[https://en.wikipedia.org/wiki/Ehrenfest\\_theorem](https://en.wikipedia.org/wiki/Ehrenfest_theorem)

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi dx = \int_{-\infty}^{\infty} (\hat{A} \Psi)^* \Psi dx \quad (24)$$

A useful property of a Hermitian operator is that it is a complex commutator with respect to our complex conjugates  $\Psi^*$  and  $\Psi$ , meaning that it can be moved left of  $\Psi^*$  in the particular was shown in (24).

$$\hat{A} \Psi = a \Psi \quad (25)$$

Another useful postulate:

The sole immediate result of an individual measurement of  $A$  will be the **eigenvalue**  $a$  of  $\hat{A}$

This postulate naturally leads to the conclusion in (25).

$$\langle A \rangle = \langle \Psi | \hat{A} \Psi \rangle = \langle \hat{A} \Psi | \Psi \rangle \quad (26)$$

Finally, Hermitian operators play very nicely with bra-ket notation, as we see in (26).

## 5.5 The Hamiltonian Operator

$$\hat{H} = \frac{-\hbar^2}{2m} \nabla^2 + V(x) \quad (27)$$

Oftentimes, it is necessary to simplify the notation in Schrödinger's equation – to do this, we can use the **Hamiltonian operator**  $\hat{H}$ , which is defined in (27). Note that  $\hat{H}$  represents one side of Schrödinger's equation without  $\Psi(x, t)$ , as seen previously in (9).

$$\hat{H} \psi = E \psi \quad (28)$$

In addition to this, note that this operator represents the amount of *energy* in the system, as it has an eigenvalue  $E$ .

## 6 Heisenberg's Uncertainty Principle

When measuring the position of a subatomic particle with high precision, we unfortunately are unable to measure its momentum with a similarly high precision. The reason for this is due to the fact that the instruments with which we measure this particle are themselves affecting the particle's behavior, leading to this *uncertainty*.

$$\sigma_p \sigma_x \geq \frac{\hbar}{2} \quad (29)$$

To mathematically model the limits of our measuring abilities, we can use equation (29), known as **Heisenberg's Uncertainty Principle**<sup>11</sup> as our guideline.

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<sup>11</sup>[https://en.wikipedia.org/wiki/Heisenberg%27s\\_uncertainty\\_principle](https://en.wikipedia.org/wiki/Heisenberg%27s_uncertainty_principle)



## 6.1 Commutators

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (30)$$

Although not strictly related to the Heisenberg Uncertainty Principle, **commutators** are a useful tool that we use in several situations in quantum mechanics, shown in (30)

## 6.2 The General Uncertainty Principle

$$\sigma_A^2 \sigma_B^2 \geq \left( \frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2 \quad (31)$$

In addition to Heisenberg's uncertainty principle, we have a more general version which can be used for all sorts of phenomena, quantum or not, shown in (31).

# 7 Solutions to Schrödinger's Equation

$$\Psi(x, t) = \psi(x)\phi(t) = \psi(x)e^{-i\frac{E}{\hbar}t} \quad (32)$$

When solving Schrödinger's equation, we can assume that the solution  $\Psi$  is separable into position-dependent and time-dependent factors, as we see in (32).

$$\Psi(x, t) = \sum_{n=1}^N c_n \Psi_n = \sum_{n=1}^N c_n \psi_n e^{-i\frac{E_n}{\hbar}t} \quad (33)$$

If we are dealing with a non-continuous (aka quantized) set of  $N$  individual solutions to our wavefunction, we can use (33) as a way to find our  $\Psi(x, t)$ .

## 7.1 Stationary States

$\psi$  is classified as a *stationary state*<sup>12</sup>, due to the fact that it is independent of time. In addition to this, we can also assume that the following is true for stationary states:

- The probability density and expectation values are constant in time
- The energy is 100% certain, such that  $\sigma_E = 0$

## 7.2 The Time-Independent Schrödinger Equation

Oftentimes, it is necessary to simplify the notation in Schrödinger's equation – to do this, we can use the **Hamiltonian operator**  $\hat{H}$ , which is defined in (27). Note that  $\hat{H}$  represents one side of Schrödinger's equation without  $\Psi(x, t)$ , as seen previously in (9).

$$E_n \psi_n = \hat{H} \psi_n \iff E_n \psi_n = \left[ \frac{-\hbar^2}{2m} \nabla^2 + V(x) \right] \psi_n \quad (34)$$

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<sup>12</sup>[https://en.wikipedia.org/wiki/Stationary\\_state](https://en.wikipedia.org/wiki/Stationary_state)

If we decide to simply work with  $\psi(x)$  rather than  $\Psi(x, t)$ , we end up having to deal with the **Time-Independent Schrödinger Equation**<sup>13</sup>, or **TISE** for short. This is shown above in (34) using both the Hamiltonian operator and the full notation.

$$\psi(x) = \sum_{n=1}^N c_n \psi_n \quad (35)$$

An important thing to note, however, is that using (34) is one of many steps needed to find  $\psi$ , since it is the sum of all quantized time-independent wavefunctions  $\psi_n$ , each with its own coefficient; this relationship is shown in (35).

**Boundary Conditions** When using the the TISE, we have that:

- $\psi$  **must** be continuous, with  $\psi = 0$  when  $|V(x)| \rightarrow \infty$
- $\nabla\psi$  **must** be continuous when  $|V(x)| < \infty$

## 7.3 Harmonic Oscillator Potentials

Locally speaking, a large portion of potentials can be approximated by a **harmonic oscillator**<sup>14</sup>

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{1}{2} m \omega^2 x^2 \psi = E \psi \quad (36)$$

Given such a potential, we end up with a TISE of the form shown in (36).

### 7.3.1 Ladder Operators

$$\hat{a}_{\pm} = \frac{1}{\sqrt{\mp i \hat{p} + m \omega \hat{x}}} \quad (37)$$

Assuming still that we have quantized states  $\psi_n$  where  $n \in \mathbb{N}$ , wouldn't it be useful to be able to find  $\psi_{n+1}$  and  $\psi_{n-1}$ ? Using the **ladder operator**<sup>15</sup> shown in (37) makes this possible.

$$[\hat{a}_-, \hat{a}_+] = \hat{a}_- \hat{a}_+ - \hat{a}_+ \hat{a}_- = 1 \quad (38)$$

Note that these operators are **non-Hermitian**, and that their commutator is equal to 1, as shown in (38). In addition to this, they have the property that the product of the minus operator and the ground state is zero, such that  $\hat{a}_- \psi_0 = 0$ .

$$\psi_{n+1} = \frac{1}{\sqrt{n+1}} \hat{a}_+ \psi_n \quad (39)$$

To increase our state, we can use (39).

<sup>13</sup>[https://en.wikipedia.org/wiki/Schr%C3%B6dinger\\_equation#Time\\_independent](https://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation#Time_independent)

<sup>14</sup>[https://en.wikipedia.org/wiki/Quantum\\_harmonic\\_oscillator](https://en.wikipedia.org/wiki/Quantum_harmonic_oscillator)

<sup>15</sup>[https://en.wikipedia.org/wiki/Ladder\\_operator#Harmonic\\_oscillator](https://en.wikipedia.org/wiki/Ladder_operator#Harmonic_oscillator)

$$\psi_{n-1} = \frac{1}{\sqrt{n}} \hat{a}_- \psi_n \quad (40)$$

To lower our state, we can use (40).

$$\psi_n = A_n \hat{a}_+^n \psi_0 \quad (41)$$

Given a ground state  $\psi_0$ , we can find any state  $\psi_n$  by repeating (39) over and over until we reach our desired  $n$ ; to simplify this process, we can also perform this in one step, shown in (41).

### 7.3.2 Ground States

$$\psi_0 = C e^{-\frac{m\omega}{2\hbar} x^2} \quad (42)$$

We can easily find the ground state  $\psi_0$  for our time independent wavefunction  $\psi$  via the usage of (42).

### 7.3.3 Energy

$$\hat{H} = \hbar\omega \left( \hat{a}_+ \hat{a}_- + \frac{1}{2} \right) \quad (43)$$

We can redefine the Hamiltonian operator in terms of our ladder operators, as shown in (43).

$$E_n = \hbar\omega \left( n + \frac{1}{2} \right), \text{ for } n \in \mathbb{N} \quad (44)$$

Using our redefined  $\hat{H}$ , we can use its eigenvalue to find the energy  $E_n$  of a particular state via (44).

### 7.3.4 Dimensionless TISE

$$\frac{d^2\psi(\xi)}{d\xi^2} = (\xi^2 - K) \psi(\xi), \text{ for } \xi = \sqrt{\frac{m\omega}{\hbar}} x \text{ and } K = 2 \frac{E}{\hbar\omega} \quad (45)$$

If we wish, we can rewrite our time-independent Schrödinger equation for a harmonic oscillator to be dimensionless (aka without units) by using the redefinition shown in (45).

$$\psi(\xi) = h(\xi) e^{-\frac{1}{2}\xi^2} \quad (46)$$

$$h(\xi) = \sum_j a_j \xi^j, \text{ with } a_{j+2} = \frac{2j - K + 1}{(j+2)(j+1)} a_j \quad (47)$$

The analytical solution to our HO TISE is then shown in (46), with its function  $h(\xi)$  defined for us in (47). Since we can only find  $a_{j+2}$  using the above equations, it is obvious that we will be in need of two initial conditions, ie both  $a_0$  and  $a_1$ ; the solutions stemming from these are called *even* and *odd*, respectively.

Fortunately, we have a boundary condition stating that *either*  $a_0$  or  $a_1$  must be equal to zero, and that the series must end at  $j_{\max} = n$  and  $K = 2n + 1$ , with  $n$  being the state of our current wavefunction  $\psi_n$ .

### 7.3.5 Analytical Solution

$$\psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{1}{2}\xi^2} \quad (48)$$

The generalized analytical solution for the HO TISE can be found via the usage of a **Hermite Polynomial**<sup>16</sup> in (48), where we assume that  $\xi$  is defined the same as in (45).

## 7.4 Bound and Unbound States

Through earlier mechanics courses, we are all familiar with the concept of *classical* bound and unbound states – a classical bound state is simply one where a particle or object cannot escape a potential well, either due to not having enough energy to get over a bump, or due to the fact that the well is infinitely deep. A classical unbound state is one where our object will fall endlessly (in one dimension, it's as though the object will move away forever into the infinity of the x-axis).

For quantum mechanics, we must change our perspective slightly – the difference here is that we must consider the possibility of **Quantum Tunneling**<sup>17</sup>, whereby a particle may be able to get through a potential bump even though it is technically "in the way."

Mathematically speaking, our quantum bound state will always have an energy  $E < V(\infty)$  and  $E < V(-\infty)$ , while everything else is considered unbound!

### 7.4.1 Continuous Energy Distributions

Previously, we've been dealing strictly with quantized energy, but only because we've only been exposed to bound states! When dealing with *unbound* states, we must consider that our energy is now continuous, and that we cannot simply use the solutions given in these previous sections – instead, we will need to introduce the continuous TISE wavefunction  $\phi(k)$ , which is the continuous equivalent to  $\psi(x)$ .

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \omega(k)t)} dk \quad (49)$$

Since the purpose of finding our  $\psi(x)$  was generally with the intent to find our  $\Psi$ , we must find an analogous solution for our continuous  $\phi(k)$ ; this is given in (49).

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \Psi(x, 0) dx \quad (50)$$

Conversely, if we are given the initial condition for TDSE wavefunction  $\Psi(x, 0)$ , we can use it to our advantage and find our  $\phi(k)$ , as seen in (50).

<sup>16</sup>[http://physics.gmu.edu/~dmaria/590%20Web%20Page/public\\_html/qm\\_topics/harmonic/](http://physics.gmu.edu/~dmaria/590%20Web%20Page/public_html/qm_topics/harmonic/)

<sup>17</sup>[https://en.wikipedia.org/wiki/Quantum\\_tunneling](https://en.wikipedia.org/wiki/Quantum_tunneling)

Note that these equations require the usage of  $k$  and  $\omega(k)$ , which were discussed earlier in Section 2.

## 7.5 Non-Normalizeable Free Particle Plane Wave Solutions

$$\psi_k(x) = Ae^{ikx} + Be^{-ikx}, \text{ where } E = \frac{\hbar^2 k^2}{2m} \quad (51)$$

Even if our free particle plane wave solutions is non-normalizeable, we can still use it as an approximation for a particle with a sharp energy, as shown in (51).

In addition to this, the direction in which a plane wave is moving depends on the sign before  $k$  in the exponent. A negative sign means it is going left, and a positive means it is going right.

## 8 The Finite Well

Up to this point, we have been working mostly with *infinite* potential wells, which result in strictly bound states. Now that we are generalizing many of the aforementioned concepts for a *finite* potential well, we will be dealing both with bound and unbound states.

$$V(x) = \begin{cases} -V_0 & \text{for } -a \leq x \leq a \\ 0 & \text{otherwise} \end{cases} \quad (52)$$

A *finite* potential well, where there is a small potential drop in the range  $\pm a$ , has a potential like the one shown in (52).

Given a finite potential well and a bound state, it is the case that the energy is quantized, meaning that it must be calculated numerically – the reasons for this will be explained further.

### 8.1 Bound States

In general, we know that bound states have an energy  $E < 0$  when we set the energy level based on the potential at  $-a \leq x \leq a$ . In addition, this means that we have a symmetric potential, which can result in two types of solutions: symmetrical and antisymmetrical solutions.

Since we have three separate locations in mind (before the well, in the well, after the well) we must solve the TISE for all three locations. In essence, what we can do first is determine what  $\Psi$  and  $\nabla\Psi$  is within the well, and then use their values on the edge of the well as the initial conditions for our two other locations.

Once this is done, we can find an equation for the quantized values of  $E$ , which must be solved numerically.

### 8.2 Reflection and Transmission

Since we are dealing with a finite well, we can no longer assume that our wavefunction is reflected perfectly when it hits one of the walls of the well – instead, we now must manually calculate

what portion of the wave is **reflected**<sup>18</sup> and what portion is **transmitted**<sup>19</sup>.

$$R = \frac{|B|^2}{|A|^2} \quad (53)$$

$$T = \frac{|F|^2}{|A|^2} \quad (54)$$

For an incoming wave of the form  $Ae^{ikx}$ , we can find the reflected wave  $Be^{-ikx}$  via (53), and the transmitted wave via (54).

$$R(E) + T(E) = 1 \quad (55)$$

Something important thing to realize is that it is not possible for the sum of the reflected and transmitted wavefunctions to be greater than the original wavefunction, leaving us with (55) as a mathematical representation of this concept.

Generally, we can find these coefficients by using our aforementioned boundary conditions to solve for whatever variable is unknown.

Interestingly enough, the concept of **quantum tunneling** is essentially due to the fact that a portion of the wavefunction may be transmitted through a potential barrier, while a classical object would be unable to pass it.

### 8.3 The Dirac Delta

$$\delta(x) = \begin{cases} \infty & \text{for } x = 0 \\ 0 & \text{otherwise} \end{cases} \quad (56)$$

$$\int_{-\infty}^{\infty} \delta(x) dx = 1 \quad (57)$$

When dealing with a variety of natural phenomena, we will sometimes encounter situations where we have potential barriers (or wells) at specific points, but not elsewhere. For these kinds of situations, we may refer to the **Dirac delta function**<sup>20</sup>, which is a misnomer, as it is not technically a function but rather a *distribution*. Nevertheless, it is defined in (56), with a valuable and important constraint defined in (57).

### 8.4 Delta Potentials

$$V(x) = -\alpha\delta(x) \quad (58)$$

It is important to note that we can have both bound and unbound states when dealing with a  $\delta$  potential<sup>21</sup> [such as the one shown in (58)] depending on whether the total energy in the system is larger than zero or not (assuming that we set zero to be the energy outside the well.)

<sup>18</sup>[https://en.wikipedia.org/wiki/Reflection\\_coefficient](https://en.wikipedia.org/wiki/Reflection_coefficient)

<sup>19</sup>[https://en.wikipedia.org/wiki/Transmission\\_coefficient](https://en.wikipedia.org/wiki/Transmission_coefficient)

<sup>20</sup>[https://en.wikipedia.org/wiki/Dirac\\_delta\\_function](https://en.wikipedia.org/wiki/Dirac_delta_function)

<sup>21</sup>[https://en.wikipedia.org/wiki/Delta\\_potential#Single\\_delta\\_potential](https://en.wikipedia.org/wiki/Delta_potential#Single_delta_potential)

$$\Delta(\nabla\psi(x)) = \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \nabla^2\psi dx \quad (59)$$

An important thing to note when dealing with  $\delta$  potentials, is the fact that  $\psi(x)$  *must* be continuous for it to be valid. We may however choose to determine the measure of discontinuity in  $\nabla\psi(x)$ , which we can accomplish through (59).

## 9 The 5 Postulates of Quantum Mechanics

In the course of this guide, we've been through a number of concepts – everything, however, is constructed upon a small set of five postulates (or axioms). This section will be a summary of the most valuable

### 9.1 Postulate 1

$$\hat{H}\Psi = i\hbar \frac{\partial}{\partial t} \Psi \quad (60)$$

The state of a system is based on the wavefunction  $\Psi(x, t)$ , which is a solution of the time-dependent Schrödinger equation (60), where  $\hat{H}$  is the systems *Hamiltonian operator*.

$\Psi(x, t)$  contains *all* the information about this system.

#### Comments

1. We can freely multiply  $\Psi$  with a constant – this is useful when taking normalization into account!

$$\langle \psi_i | \psi_j \rangle = \int_{-\infty}^{\infty} \psi_i^* \psi_j dx \quad (61)$$

2. The solution to the Schrödinger equation can be represented by abstract vectors  $|\psi\rangle$ , which exist in a complex inner product space defined in (61). This is known as Bra-Ket notation (invented by Dirac), which are vectors in a *Hilbert space*.

### 9.2 Postulate 2

For every observable  $Q$ , there exists a linear Hermitian operator  $\hat{Q}$ .

#### Comments

$$\hat{Q}(a\psi_i + b\psi_j) = a\hat{Q}\psi_i + b\hat{Q}\psi_j \quad (62)$$

1. Such operators being linear leads to the implication shown in (62).

$$\int_{-\infty}^{\infty} \psi_i^* \hat{Q}\psi_j dx = \int_{-\infty}^{\infty} (\hat{Q}\psi_i)^* \psi_j dx \iff \langle \psi_i | \hat{Q}\psi_j \rangle = \langle \hat{Q}\psi_i | \psi_j \rangle \quad (63)$$

2. Such operators are also Hermitian, as shown in (63).
3. The *canonical variables* are  $x$  and  $p$ , with  $\hat{x} = x$ , and  $\hat{p} = -i\hbar\nabla$ .
4. These operators are linear transformations for vectors in a vector space.

### 9.3 Postulate 3

$$\hat{Q}\psi_n = q_n\psi_n \iff \hat{Q}|\psi_n\rangle = q_n|\psi_n\rangle \quad (64)$$

The *only* possible result of measuring an observable  $Q$ , is the eigenvalue  $q_n$  of the operator  $\hat{Q}$ , such as in (64).

#### Comments

1. Immediately after the measurement of  $q_n$ , a system's state is equal to  $\psi_n$  – this is known as the collapse of a wavefunction.
2. The set  $\{q_n\}$  is called the operator's spectrum; it can be *finite*, *countably infinite*, or *uncountably infinite*.
3. If multiple eigenstates<sup>22</sup> have the same eigenvalues, then the eigenvalue is *degenerate*<sup>23</sup>. The number of states that are degenerate is called the *degree of degeneration*  $d(n)$ .

$$c_n = \int_{-\infty}^{\infty} \psi_n^* \psi dx = \langle \psi_n | \psi \rangle \quad (65)$$

4. The probability of measuring the  $n^{\text{th}}$  eigenvalue for a state  $\psi = \sum c_n \psi_n$  is  $|c_n|^2$ , where  $\sum |c_n|^2 = 1$ ;  $c_n$  can be found via Fourier's trick, shown in (65).

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0 \quad (66)$$

5. Operators whose commutator is equal to zero [seen in (66)] have the same eigenfunctions, and are called *compatible observable*<sup>24</sup>.

$$\sigma_A^2 \sigma_B^2 \geq \left( \frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2 \quad (67)$$

6. Two incompatible commutators follow the general uncertainty principle, shown in (67)

### 9.4 Postulate 4

$$\langle Q \rangle = \langle \psi | \hat{Q} \psi \rangle = \int_{-\infty}^{\infty} \psi^* \hat{Q} \psi dx \quad (68)$$

An ensemble of systems prepared in the state  $|\psi\rangle$  will have an expectation value as shown in (68).

<sup>22</sup>[https://en.wikipedia.org/wiki/Introduction\\_to\\_eigenstates](https://en.wikipedia.org/wiki/Introduction_to_eigenstates)

<sup>23</sup>[https://en.wikipedia.org/wiki/Degenerate\\_energy\\_levels](https://en.wikipedia.org/wiki/Degenerate_energy_levels)

<sup>24</sup>[https://en.wikipedia.org/wiki/Complete\\_set\\_of\\_commuting\\_observables](https://en.wikipedia.org/wiki/Complete_set_of_commuting_observables)



**Comments**

$$\sigma_Q^2 = \left\langle (Q - \langle Q \rangle)^2 \right\rangle = \langle Q^2 \rangle - \langle Q \rangle^2 \quad (69)$$

1. The variance is defined in (69)
2. If we have that  $\sigma_Q = 0$ , then  $Q$  is known with 100% certainty.

**9.5 Postulate 5**

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle \quad (70)$$

If  $\hat{Q}$  is a Hermitian operator, and the set  $\{|\psi_n\rangle\}$  is the set of *all* eigenstates for  $\hat{Q}$ , then (70) is a complete set.

**Comment** For continuous eigenvalues, we have that  $\langle \psi_n | \psi_m \rangle = \delta_{m,n}$ .