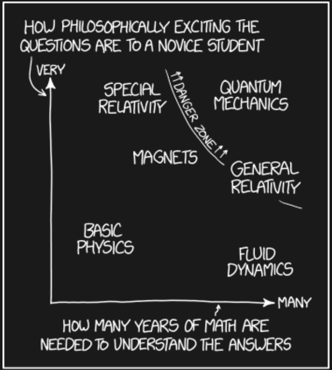
Module 2.1 - Introduction to Quantum Mechanics

History, Formalism, Concepts and Simulations

Rajeshkumar Vivan Bhatt

Horizon IITM, CFI

CFI Summer-School, 2021



WHY SO MANY PEOPLE HAVE WEIRD IDEAS ABOUT QUANTUM MECHANICS

Structure

1. History
2. Mathematical Introduction
3. Basics of Quantum Mechanics
4. Applications of Schrödinger equation
5. Visualisations

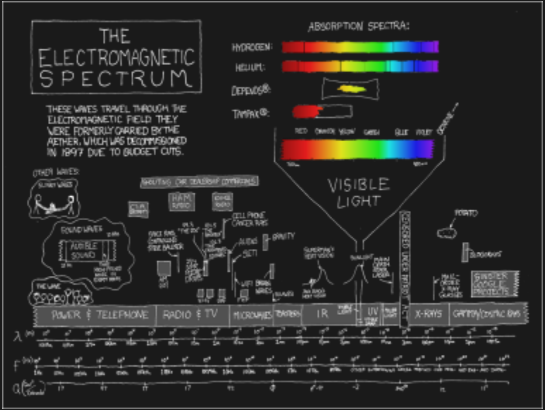
1 History

2 Mathematical Introduction

3 Basics of Quantum Mechanics

4 Applications of Schrödinger equation

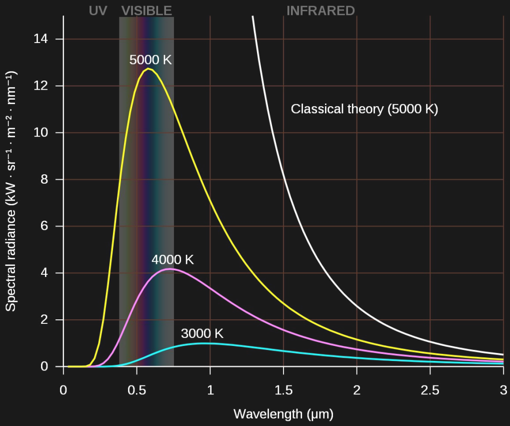
Where it all started



Ultraviolet Catastrophe

Blackbody Radiation

- What is a blackbody?
- Spectral radiance from stat mech: $B_\lambda(T) = \frac{2ck_BT}{\lambda^4}$



Ad hoc quantization?

- "Phase Space" - TBT PH1010
- Planck's hypothesis :

$$E = \frac{hc}{\lambda}$$

- New spectral distribution function:

$$B_\lambda(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$

- Cheap trick v/s physical implication
- Ensemble of Photons
- Photoelectric effect and 1921 Nobel

Photoelectric effect

Classical Predictions

- Continuous light waves
- Accumulation of energy
- Increase in stopping voltage with intensity
- Delayed emission for dim light

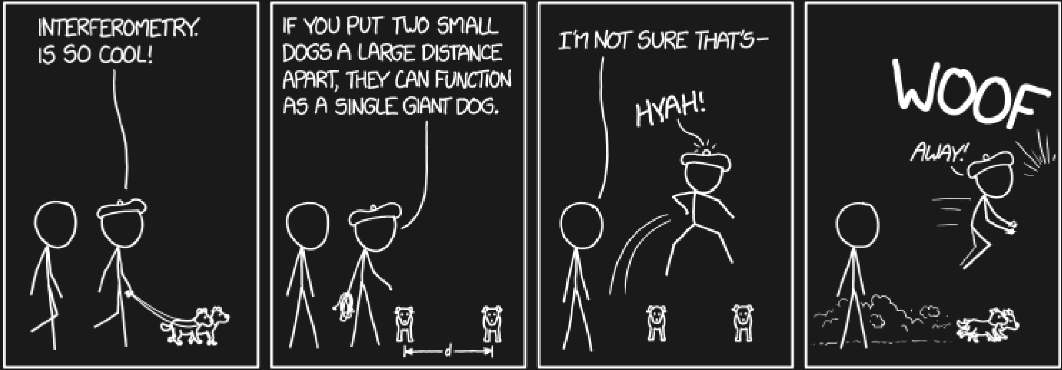
Observations

- ??
- Immediate emission
- Increase in current with intensity
- Emission only after a particular frequency

Light Quanta

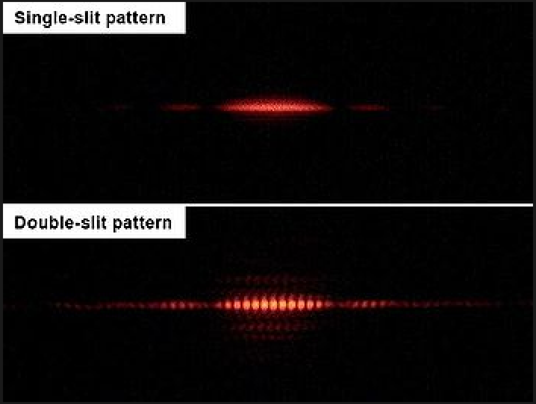
$$KE_{max} = h\nu - \phi_o$$

Waves for dummies



Double slit experiment

- Young's Interference pattern
- Observation
- Single particle interference
- Feynman's thoughts



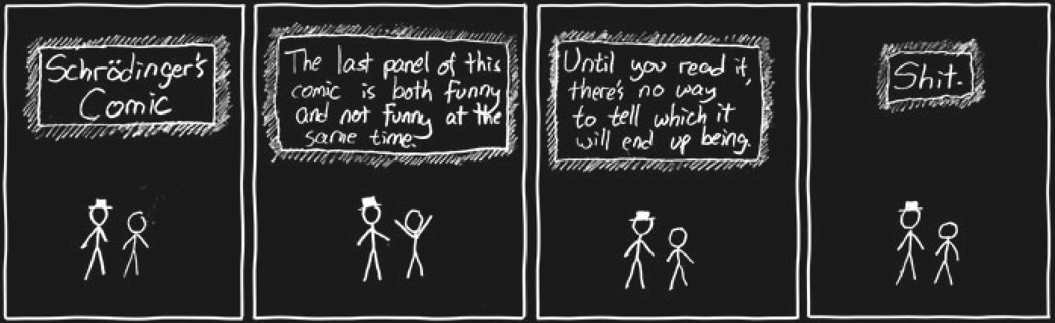
De Broglie Hypothesis

- Extending Einstein's theory to matter
- De Broglie wavelength given by:

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

- Experimental verification
- Group velocity
- "Matter wave" and the Schrödinger equation

Schrödinger



Schrödinger Equation

Time dependent equation:

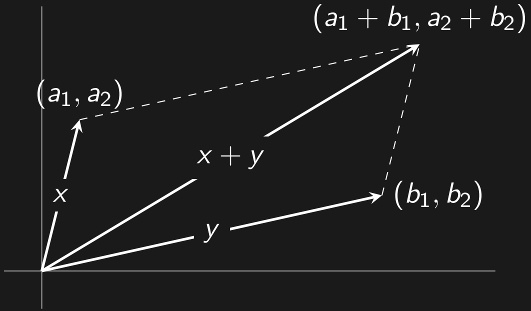
$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

Time independent equation:

$$\hat{H}|\Psi(t)\rangle = E|\Psi(t)\rangle$$

High-School Vectors

- Have **magnitude** and **direction**.
- Follow **Parallelogram Law of Addition**.
- Has defined **Scalar** and **Vector** product.
- Contrasted with **scalars**.




WE NEED TO GO
DEEPER

Fields

From other fields

Figure: Field of a biologist

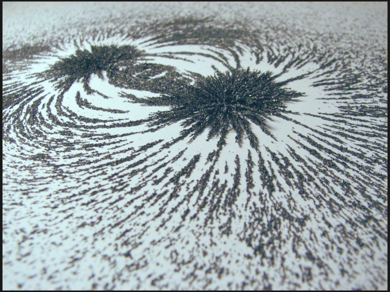


Figure: Field of a physicist

Fields

From mathematics

- A **Field** is a set which is closed under operations "addition" and "multiplication" (along with some other conditions).
- Elements of a field are known as *scalars*.

Fields

Formal definition

Definition (Field)

A field $\mathbb{F}$ is a set on which two operations $+$ and $\cdot$ are defined such that $x + y \in \mathbb{F} \, \forall \, x, y \in \mathbb{F}$, and the following hold true for all $a, b, c \in \mathbb{F}$:

1. $a + b = b + a$ and $a \cdot b = b \cdot a$ (commutativity of $+$ and $\cdot$)
2. $(a + b) + c = a + (b + c)$ and $(a \cdot b) \cdot c = a \cdot (b \cdot c)$ (associativity of $+$ and $\cdot$)
3. $\exists! \, 0, 1 \in \mathbb{F} \ni 0 + a = a$ and $1 \cdot a = a$ (existence of identity elements for $+$ and $\cdot$)
4. $\forall \, a \in \mathbb{F}$ and $\forall \, b \neq 0 \in \mathbb{F} \, \exists \, c, d \in \mathbb{F} \ni a + c = 0$ and $b \cdot d = 1$ (existence of inverses for $+$ and $\cdot$)
5. $a \cdot (b + c) = a \cdot b + a \cdot c$ (compatibility of $+$ and $\cdot$)

Examples of Fields

- The set of real numbers $\mathbb{R}$ (with the usual addition and multiplication)
- The set of rational numbers $\mathbb{Q}$ (with the usual addition and multiplication)
- The set of complex numbers $\mathbb{C}$ (with the usual addition and multiplication)
- The binary field $\mathbb{F}_2 = \{0, 1\}$ with the following definitions for $+$ and $\cdot$:

$+$	0	1
0	0	1
1	1	0

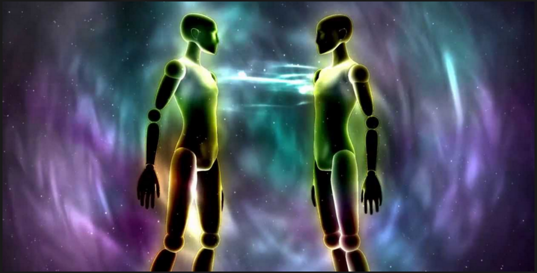
$\cdot$	0	1
0	0	0
1	0	1

NOT Example of Fields

- The set of natural numbers $\mathbb{N}$
- The set of integers $\mathbb{Z}$

NOT Example of Fields

- The set of natural numbers $\mathbb{N}$
- The set of integers $\mathbb{Z}$
- Whatever abomination this is:



Vector Spaces

Formal Definition

Definition (Vector Space)

A **Vector Space** V over a field $\mathbb{F}$ is a set on which two operations **addition** and **scalar multiplication** are defined such that the set is *closed* under both the operations, and the following conditions hold ($\forall\, \mathrm{x}, \mathrm{y}, \mathrm{z} \in \mathrm{V}$ and $\forall\, a, b \in \mathbb{F}$):

1. $\mathrm{x} + \mathrm{y} = \mathrm{y} + \mathrm{x}$
2. $(x + y) + z = x + (y + z)$
3. $\exists\, 0 \in \mathrm{V} \ni \mathrm{x} + 0 = \mathrm{x}, \forall\, \mathrm{x} \in \mathrm{V}$
4. $\forall\, \mathrm{x} \in \mathrm{V}, \exists\, \mathrm{y} \in \mathrm{V} \ni \mathrm{x} + \mathrm{y} = 0$

Vector Spaces (cont.)

Formal Definition

5. $\forall\, \mathrm{x} \in \mathrm{V},\ 1\mathrm{x} = \mathrm{x}$
6. $(ab)\mathrm{x} = a(b\mathrm{x})$
7. $a(\mathrm{x} + \mathrm{y}) = a\mathrm{x} + a\mathrm{y}$
8. $(a + b)\mathrm{x} = a\mathrm{x} + b\mathrm{x}$

The elements of the vector space are known as **vectors**.

NOTE

The term "vectors" now represent any element of a vector space, and is not limited to the notion of vectors which is taught in high-school or outside mathematics.

Takeaways

From vector-spaces

- A vector space is a *set with two defined operations satisfying some conditions*
- Every vector space is defined over some given field. The operations and discussions about a vector space imply its dependence on whatever field the vector space is defined upon.

Examples of Vector-Spaces

1. The set of all **n-tuples** over a field $\mathbb{F}$ is a vector space F^n with the operations defined as element-wise addition and scalar-multiplication, that is: If $\mathrm{x} = (x_1, x_2, \dots x_n)$ and $\mathrm{y} = (y_1, y_2, \dots y_n)$ are two elements in F^n, then:
   - $\mathrm{x} + \mathrm{y} = (x_1 + y_1, x_2 + y_2, \dots, x_n + y_n)$, and
   - $a\mathrm{x} = (ax_1, ax_2, \dots, ax_n)$
2. The set of all $m \times n$ matrices from a field $\mathbb{F}$ is a vector space denoted by $\mathrm{M}_{m\times n}(\mathbb{F})$, with the operations matrix addition and scalar multiplication, that is: For $\mathrm{A}, \mathrm{B} \in \mathrm{M}_{m\times n}(\mathbb{F})$ and $c \in \mathbb{F}$,
   - $(\mathrm{A} + \mathrm{B})_{ij} = \mathrm{A}_{ij} + \mathrm{B}_{ij}$, and
   - $(c\mathrm{A})_{ij} = c\mathrm{A}_{ij}$
3. The set of all polynomials with coefficients from a field $\mathbb{F}$ is a vector space $\mathrm{P}(\mathbb{F}) = \{f(x) = \sum_{i=0}^{n} a_i x^i \mid a_i \in \mathbb{F} \, \forall \, i\}$

Subspaces

Formal definition

Definition (Subspace)

A subset W of a vector space V over a field $\mathbb{F}$ is said to be a subspace of V, if W is a also a vector space over $\mathbb{F}$ with the addition and scalar multiplication operators same as defined on V.

For any vector space V, there are two trivial subspaces: V and $\{0\}$.

Necessary condition for subspaces

By using the conditions for a vector space, and using the properties of subsets, the following conditions can be drawn for a subset to be a subspace. Note that these are necessary *and* sufficient conditions, and any set not obeying these cannot be a subspace.

Theorem

Let V *be a vector space over field* $\mathbb{F}$ *and let* W *be a subset of* V. *Then* W *is a subspace of* V *if and only if the following conditions hold for the operations defined on* V*:*

1. $0 \in \mathrm{W}$
2. $x + y \in \mathrm{W} \; \forall \, x, y \in \mathrm{W}$
3. $cx \in \mathrm{W} \; \forall \, x \in \mathrm{W}$ *and* $a \in \mathbb{F}$

Necessary condition for subspaces (cont.)

Proof.

Case 1: $\mathbb{W}$ is a vector space. Then 2 and 3 hold due to the definition of a vector space. Now, there exists a vector $0'$ in $\mathbb{W}$ such that $x + 0' = x$ for all elements in $\mathbb{W}$. But we also have $x + 0 = x$ for all elements in $\mathbb{V}$ (and hence $\mathbb{W}$). Therefore $0' = 0$. This proves 1.

Case 2: The conditions hold. (Left as an exercise to the reader.) □

Example of Subspaces

1. The set of all symmetric $n \times n$ matrices is a subspace of $\mathrm{M}_{n\times n}(\mathbb{F})$.
2. Let S be a non-empty set, and $\mathbb{F}$ be any field. Let $\mathcal{F}(S, \mathbb{F})$ be the set of all functions from S to $\mathbb{F}$. The set $\mathcal{F}(S, \mathbb{F})$ is a vector space (how ?). Now, let $\mathcal{C}(\mathbb{R})$ denote the set of all continuous real-valued functions defined on $\mathbb{R}$. $\mathcal{C}(R)$ is a subspace of $\mathcal{F}(\mathbb{R}, \mathbb{R})$. (how ?)
3. An $m \times n$ matrix A with $\mathrm{A}_{ij} = 0$ whenever $i < j$ is known as a **lower triangular** matrix. The set of all lower triangular matrices is a subspace of $\mathrm{M}_{m\times n}(\mathbb{F})$.

Linear Combinations and Span

As the name implies.

Definition (Linear combination)

Let V be a vector space over $\mathbb{F}$ and let $S = \{\mathrm{u}_1, \ldots, \mathrm{u}_n\}$ be a non-empty subset of V. A vector $\mathrm{v} \in \mathrm{V}$ is said to be a **linear combination** of vectors of S, if there exists $a_1, a_2, \ldots, a_n \in \mathbb{F}$ such that $\mathrm{v} = \sum_{i=0}^{n} a_i \mathrm{u}_i$

Examples:

- Consider the vector space of R^3 over R. $(4, 0, 4)$ is a linear combination of $\{(1, 0, 0), (0, 0, 2)\}$ as $(4, 0, 4) = 4(1, 0, 0) + 2(0, 0, 2)$.

Linear Combinations and Span (cont.)

- Consider the vector space $\mathrm{P}_3(\mathbb{R})$ of all polynomials of degree not exceeding 3 with coefficients from $\mathbb{R}$. Let $S = \{x^3 + 2x^2 - x + 1, x^3 + 3x^2 + 1\}$ be a subset of the vector space. Then, $x^3 - 3x + 5$ is a linear combination of S.
- Consider a subset $S = \{\left(\begin{smallmatrix} 0 & 2 \\ 1 & 1 \end{smallmatrix}\right), \left(\begin{smallmatrix} 3 & 0 \\ 1 & 1 \end{smallmatrix}\right)\}$ of the vector space $M_{2\times 2}(\mathbb{R})$. Now $\left(\begin{smallmatrix} -3 & 4 \\ 1 & 1 \end{smallmatrix}\right)$ is a linear combination of S.
- Consider the vector space of all continuous functions $\mathcal{C}(\mathbb{R})$. Let $S = \{\sin x, \cos x\}$ be a subset of $\mathcal{C}(\mathbb{R})$. e^x is **not** a linear combination of S. (why not?)

Linear Combinations and Span (cont.)

An important concept associated with linear combinations is the **span** of a set (or subset for that matter).

Definition (Span)

Let S be a non-empty subset of a vector space V over $\mathbb{F}$. The **span** of S is defined as the set of all linear-combinations of the vectors in S, denoted by $\mathrm{span}(S)$. According to the Empty sum convention, $\mathrm{span}(\emptyset) = \{0\}$.

Now that we have seen subsets and spans, we can combine both concepts to arrive at a theorem which proves to be very useful for deriving other results in linear algebra.

Linear Combinations and Span (cont.)

Theorem

The span of a subset S of a vector space V is a subspace of V. Also, if W is a subspace of V such that $S \subseteq \mathrm{W}$ then span$(S) \subseteq \mathrm{W}$.

Proof.

Case 1: $S = \emptyset$. In this case we have span$(\emptyset) = \{0\}$, which is a subspace of any vector space. So the theorem is true.

Case 2: $S \neq \emptyset$. In this case, S is non-empty, and contains an element, say z. We have $0\mathrm{z} = 0 \in$ span(S). Now, let $\mathrm{x}, \mathrm{y} \in$ span(S). Then, there exists vectors

Linear Combinations and Span (cont.)

$u_1, u_2, \ldots, u_m, v_1, v_2, \ldots, v_n \in S$, and scalars $a_1, a_2, \ldots, a_m, b_1, b_2, \ldots, b_n \in \mathbb{F}$ such that

$$x = \sum_{i=0}^{m} a_i u_i, \text{ and } y = \sum_{i=0}^{n} b_i v_i$$

Then we have

$$x + y = \sum_{i=0}^{m} a_i u_i + \sum_{i=0}^{n} b_i v_i, \text{ and } cx = \sum_{i=0}^{m} (ca_i) u_i \tag{1}$$

From (1), and the earlier result that $0 \in \text{span}(S)$ we have that $\text{span}(S)$ is a subspace of $\mathbb{V}$.

Linear Combinations and Span (cont.)

Consider $\mathrm{w} \in \mathrm{span}(S)$ such that $\mathrm{w} = \sum_{i=0}^{k} c_i \mathrm{w}_i$ for some vectors $\mathrm{w}_i \in S$ and scalars $c_i \in \mathbb{F}$. Since $S \subseteq \mathrm{W}, \mathrm{w}_i \in \mathrm{W}\ \forall\ i$ and therefore any linear combination of the w_i's is in W. Therefore $\mathrm{w} \in \mathrm{W}$. This implies $\mathrm{span}(S) \subseteq \mathrm{W}$.

$\square$

Following will be a definition which will prove useful for discussing bases in the coming parts.

Definition

A subset S of a vector space V is said to **generate** or **span** V if $\mathrm{span}(S) = \mathrm{V}$.

Linear Combinations and Span (cont.)

Examples of generating/spanning sets:

- The set $B = \{(1,1,0),(1,0,1),(0,1,1)\}$ spans the vector space R^3
- The matrices $\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$, *and* $\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$ generate $\mathrm{M}_{2\times 2}(\mathbb{R})$.

Linear (in)dependence

Another concept which complements and builds upon the linear combination, is the linear dependence of vectors.

Definition (Linear dependence)

A subset S of a vector space V is said to be **linearly dependent** if there exists finite number of distinct vectors u_i's $\in S$ and scalars a_i, not all of which are zero, such that

$$a_1\mathrm{u}_1 + a_2\mathrm{u}_2 + \ldots + a_n\mathrm{u}_n = 0 \tag{2}$$

Examples: The vectors $(1, 3)$ and $(2, 6)$ from R^2 are linearly dependent because $2(1, 3) - 1(2, 6) = (0, 0)$.

Linear (in)dependence (cont.)

With similar grounds,

Definition

A subset S of a vector space V is said to be **linearly independent** if it not linearly dependent.

Example: The vectors $(1, 0)$ and $(0, 1)$ from R^2 are linearly independent as the representation $a(1, 0) + b(0, 1) = (0, 0)$ is valid only for the trivial case of $a = 0$ and $b = 0$.

Linear (in)dependence (cont.)

Some important points to note:

- $\emptyset$ is linearly independent as linearly dependent sets must be non-empty.
- A singleton set with non-zero element is linearly independent.
- A set is linearly independent if and only if representation of 0 as the linear combination of the set are trivial representations.

Bases and Dimensions

Bases and Dimensions (cont.)

Definition

A **basis** β for a vector space V is a *linearly independent* subset of V that generates/spans V. If β is a basis for V then the vectors of β are said to form a basis for V.

Examples:

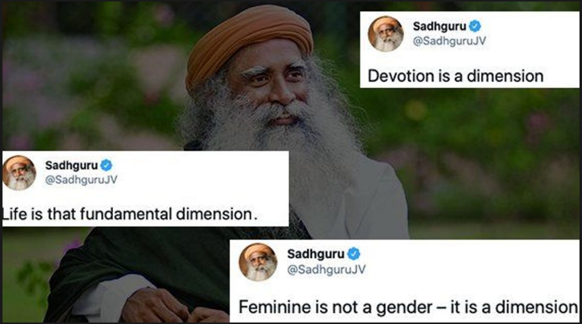
- $\emptyset$ is the basis for the zero vector space $\{0\}$.
- In F^n, consider $e_1 = (1, 0, \ldots, 0), e_2 = (0, 1, \ldots, 0), \ldots, e_n = (0, 0, \ldots, 1)$. The set $\beta = \{e_1, e_2, \ldots, e_n\}$ is the **standard basis** or **canonical basis** or **natural basis** for F^n.

Bases and Dimensions (cont.)

- The set $\{1, x, x^2, \ldots, x^n\}$ is a **standard basis** for $\mathrm{P}_n(\mathbb{F})$. For $\mathrm{P}(\mathbb{F})$, the standard basis is $\{1, x, x^2, x^3, \ldots\}$.
- The set $\{E^{11}, E^{12}, \ldots, E^{mn}\}$ is the basis for the vector space $\mathrm{M}_{m\times n}(\mathbb{F})$, where E^{ij} is the $m \times n$ matrix with a 1 in its ith row and jth column, and zero everywhere else.

Bases and Dimensions (cont.)

Now that we sorted some based definitions, we can go to the *dimensionality* of vector spaces.



Bases and Dimensions (cont.)

Definition (Dimension)

A vector space V is said to be **finite-dimensional** if it has a basis consisting of finite number of vectors. The unique number of vectors in each basis for V is called the **dimension** of V and is denoted by $\dim(\mathrm{V})$. A vector space that is not finite-dimensional is said to be **infinite-dimensional**.

Examples:

- Zero vector space $\{0\}$ has dimension 0.
- The vector space $\mathrm{M}_{m\times n}(\mathbb{F})$ has dimension mn.
- The vector space $\mathrm{P}_n(\mathbb{F})$ has dimension $n+1$.

Bases and Dimensions (cont.)

Recall the discussion about **Fields**. Now, the dimension of a vector space depends upon the field it is defined over. Consider the example of the complex vector space:

- Over the field of complex numbers $\mathbb{C}$, the vector space of complex numbers has dimension **1**, since the basis is $\{1\}$.
- Over the field of real numbers $\mathbb{R}$, the vector space of complex numbers has dimension **2**, since the basis now is $\{1, i\}$.

Bases and Dimensions (cont.)

Following will be a very important theorem, encapsulating the properties of bases, and dimensions of vector spaces.

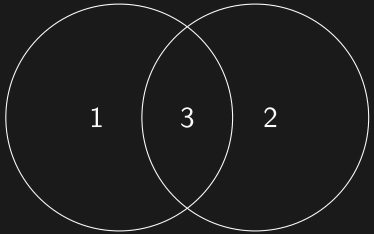
Theorem

Let $\mathbb{V}$ be a vector space with dimension n. Then,

1. *Any finite generating set for $\mathbb{V}$ contains at least n vectors, and a generating set with exactly n vectors is a basis for $\mathbb{V}$.*
2. *Any linearly independent subset of $\mathbb{V}$ with exactly n vectors is a basis for $\mathbb{V}$.*
3. *Every linearly independent subset of $\mathbb{V}$ can be extended to a basis for $\mathbb{V}$.*

Bases and Dimensions (cont.)

The relation between **generating sets**(1), **linearly-independent sets**(2) and **bases**(3) can be summarised as:



Linear Transformation/Map/Operator

Formal definition

Definition

Let V and W be two vector spaces over $\mathbb{F}$. A function $\mathsf{T} : \mathrm{V} \to \mathrm{W}$ is said to be a **linear transformation from** V **to** W if $\forall\, \mathsf{x}, \mathsf{y} \in \mathrm{V}$ and $c \in \mathbb{F}$, we have

1. $\mathsf{T}(\mathsf{x} + \mathsf{y}) = \mathsf{T}(\mathsf{x}) + \mathsf{T}(\mathsf{y})$, and
2. $\mathsf{T}(c\mathsf{x}) = c\mathsf{T}(\mathsf{x})$

A quick check for verifying linearity of transformation is the following property, which is a summary of the definition above:

$$\mathsf{T}(a\mathsf{x} + \mathsf{y}) = a\mathsf{T}(\mathsf{x}) + \mathsf{T}(\mathsf{y}) \tag{3}$$

Examples of Linear Transformations

- Define $\mathrm{T} : \mathrm{R}^2 \to \mathrm{R}^2$ by $\mathrm{T}_x(a_1, a_2) = (a_1, -a_2)$. T is called the **reflection about** x-**axis**.
- Define $\mathrm{T} : \mathrm{R}^2 \to \mathrm{R}^2$ by $\mathrm{T}_x(a_1, a_2) = (a_1, 0)$. T is called the **projection on the** x-**axis**.
- Let $\mathrm{V} = \mathcal{C}(\mathbb{R})$, be the vector space of continuous real-valued functions defined on $\mathbb{R}$. Let $a, b \in \mathbb{R}, a < b$. Define $\mathrm{T} : \mathrm{V} \to \mathbb{R}$ by

$$\mathrm{T}(f) = \int_a^b f(t)dt, \quad \forall f \in \mathrm{V}$$

Now T is a linear transformation. (how?)

Matrix representations

Every linear transformation (over FDVS) can be represented by a matrix. There exists a one-one correspondence between matrices and linear transformations. This is one of the most important concept which quantum mechanics borrows from linear algebra.
Along same lines, the vectors themselves have matrix representations based on the basis being used. These matrices are either row or column matrices.
Before we deal with the matrix representation, we need some standardised definition for the bases of the vector spaces - you will realise why this is necessary soon enough.

Ordered Basis

Definition (Ordered basis)

Let V be a FDVS. An **ordered basis** for V is a basis endowed with a specific order.

Note that the "order" in ordered-basis does not have any relation to the notion of ordered set - here the word 'order' just points to the (literal) order in which the base vectors are specified.

Examples:

- For the vector space F^n, $\beta = \{e_1, e_2, \ldots, e_n\}$ is the **standard ordered basis** or **canonical basis**.
- For the vector space $\mathrm{P}_n(\mathbb{F})$, the set $\beta = \{1, x, x^2, \ldots, x^n\}$ is the **canonical basis**.

Coordinate vectors

This is the matrix representation for the vectors themselves. **Definition:**
Let $\beta = \{u_1, u_2, \ldots, u_n\}$ be an ordered basis for the FDVS V over $\mathbb{F}$. For any $x \in \mathrm{V}$, there exists scalars $a_i \in \mathbb{F}$ such that

$$x = \sum_{i=1}^{n} a_i u_i$$

Coordinate vectors (cont.)

Now, we define the **coordinate vector of** x **relative to** β, denoted by $[\mathrm{x}]_\beta$, by

$$[\mathrm{x}]_\beta = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

Important points:

- By this definition, $[\mathrm{u}_i]_\beta = e_i$
- The correspondence $\mathrm{x} \to [\mathrm{x}]_\beta$ is a linear transformation from V to F^n

Coordinate vectors (cont.)

Examples:

- Let $\mathrm{V} = \mathrm{P}_2(\mathbb{R})$, and let $\beta = \{1, x, x^2\}$ be the canonical basis for V. If $f(x) = 6 + 9x - 420x^2$, then

$$[f]_\beta = \begin{pmatrix} 6 \\ 9 \\ -420 \end{pmatrix}$$

- Let V be the vector space of complex numbers over $\mathbb{R}$. The matrix representation of $\mathrm{v} = 11 + i5$ is

$$[\mathrm{x}]_\beta = \begin{pmatrix} 11 \\ 5 \end{pmatrix}$$

where the basis is $\beta = \{1, i\}$.

Matrix representation of linear transformations

Let V and W be FDVS with ordered bases $\beta = \{\mathsf{v}_1, \mathsf{v}_2, \ldots, \mathsf{v}_n$ and $\gamma = \{\mathsf{w}_1, \mathsf{w}_2, \ldots, \mathsf{w}_m$, respectively. Let $\mathsf{T} : \mathrm{V} \to \mathrm{W}$ be linear. Since the transformed vectors are part of the vector space W there exists unique scalars $a_{ij} \in \mathbb{F}$ such that

$$\mathsf{T}(\mathsf{v}_j) = \sum_{t=1}^{m} a_{ij}\mathsf{w}_i, \quad 1 \leq j \leq n.$$

Now, the **matrix representation of** T **in the ordered bases** β **and** γ is the $m \times n$ matrix A defined as $\mathsf{A}_{ij} = a_{ij}$, and written as $\mathsf{A} = [\mathsf{T}]_\beta^\gamma$. If $\beta = \gamma$, then it is written as $\mathsf{A} = [\mathsf{T}]_\beta$.

Examples:

Matrix representation of linear transformations (cont.)

- Let $T : \mathrm{R}^2 \to \mathrm{R}^2$ be the linear transformation defined by $T(a_1, a_2) = (a_1, -a_2)$. This is the reflection about x-axis transformation. Let β and γ be the canonical basis for R^2. Then

$$T(1,0) = (1,0) \qquad = 1e_1 + 0e_2$$
$$T(0,1) = (0,-1) \qquad = 0e_1 - 1e_2$$

Hence

$$[T]_\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Matrix representation of linear transformations (cont.)

- Let $\mathsf{T} : \mathrm{P}_3(\mathbb{R}) \to \mathrm{P}_2(\mathbb{R})$ be the linear transformation defined by $\mathsf{T}(f(x)) = \frac{df(x)}{dx}$. Let β and γ be respective canonical bases of the vector spaces. Then, the matrix representation of T is:

$$[\mathsf{T}]_\beta^\gamma = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$$

Properties of Linear Transformation

The arithmetics on linear transformations are defined as:

1. $(\mathsf{T}+\mathsf{U})(\mathsf{x}) = \mathsf{T}(\mathsf{x}) + \mathsf{U}(\mathsf{x})$
2. $(a\mathsf{T})(\mathsf{x}) = a\mathsf{T}(\mathsf{x})$

The same definitions are carried over to their matrix representations as well:

1. $[\mathsf{T}+\mathsf{U}]_\beta^\gamma = [\mathsf{T}]_\beta^\gamma + [\mathsf{U}]_\beta^\gamma$
2. $[a\mathsf{T}]_\beta^\gamma = a\,[\mathsf{T}]_\beta^\gamma$

With the concepts we have discussed so far, we can make an attempt at understanding dual-spaces and consequently the Hilbert space which occupies a crucial role in quantum mechanics.

With the concepts we have discussed so far, we can make an attempt at understanding dual-spaces and consequently the Hilbert space which occupies a crucial role in quantum mechanics.
But wait, there's more.


VECTORS SPACES
LINEAR MAPS
VECTOR SPACE OF LINEAR MAPS
imgflip.com

Vector space of linear transformations

Definition

Let V and W be vector spaces over $\mathbb{F}$. With the operations of addition and scalar multiplication defined earlier, the set of all linear transformations from V to W is a vector space denoted by $\mathcal{L}(\mathrm{V}, \mathrm{W})$. If $\mathrm{V} = \mathrm{W}$, then it is written as $\mathcal{L}(\mathrm{V})$.

This definition will be very useful for us to discuss **Dual spaces** which is the playground in which the mathematics of quantum mechanics is played.

Dual spaces

In essence, dual spaces are the vector space of all **linear functionals** on a vector space. Great, now another term to define:

Definition (Linear functionals)

A linear transformation from a vector space V to its own field $\mathbb{F}$ is called a **linear functional** on V.

Note that this is possible because, the fields are also vector spaces over them-self and their dimension is always 1.

Dual spaces (cont.)

With this definition of functionals, defining dual spaces becomes trivial:

Definition (Dual space)

The **dual space** of a vector space V over $\mathbb{F}$ is defined as the vector space $\mathcal{L}(\mathrm{V}, \mathbb{F})$, and denoted by V^*

Now we know that every vector space is *based*[1]. So we can define such a basis for the dual space as well.

Dual spaces (cont.)

Definition

Let V be a FDVS over $\mathbb{F}$ with ordered basis $\beta = \{\mathrm{x}_1, \mathrm{x}_2, \ldots, \mathrm{x}_n\}$. Let f_i be the functional corresponding to i-th coordinate. Then, the basis $\beta^* = \{\mathrm{f}_1, \mathrm{f}_2, \ldots, \mathrm{f}_n\}$ of V^* that satisfies $\mathrm{f}_i(\mathrm{x}_j) = \delta_{ij}$ is defined as the **dual basis** of β.

Here δ_{ij} is Kronecker delta.
How is this "dual space" going to be useful for us: the operators in quantum mechanics come from the dual space of the Hilbert Space.
Hilbert space, now that's a new term. A super concise definition of Hilbert space is **complex inner product space**. Now you know what to do.

---

[1] Please don't use this terminology anywhere unless you want to be scrutinised for being corny and imprecise.

Inner product

Definition

Let V be a vector space over $\mathbb{F}$. An **inner product** on V is a function that assigns, to each pair of vectors $\mathrm{x}, \mathrm{y} \in \mathrm{V}$, a scalar in $\mathbb{F}$. This is denoted by $\langle \mathrm{x}, \mathrm{y} \rangle$, and obeys the following conditions:

1. $\langle \mathrm{x} + \mathrm{y}, \mathrm{z} \rangle = \langle \mathrm{x}, \mathrm{z} \rangle + \langle \mathrm{y}, \mathrm{z} \rangle$
2. $\langle c\mathrm{x}, \mathrm{y} \rangle = c\langle \mathrm{x}, \mathrm{y} \rangle$
3. $\overline{\langle \mathrm{x}, \mathrm{y} \rangle} = \langle \mathrm{y}, \mathrm{x} \rangle$
4. $\langle \mathrm{x}, \mathrm{x} \rangle > 0$ if $x \neq 0$

Inner product (cont.)

Examples:

- The standard **dot** product is the inner-product for n-tuple vector spaces F^n.
- Let $\mathrm{V} = \mathcal{C}([0,1])$ be the vector space of all continuous real valued functions defined on the interval $[0,1]$. One inner product for this vector space is

$$\langle \mathrm{f}(x), \mathrm{g}(x) \rangle = \int_0^1 f(t)g(t)dt$$

Additional points

- The **norm** of a vector in an IPS is defined as $\sqrt{\langle x, x \rangle}$ and denoted by $\|x\|$
- A vector is said to be **normal** if its norm is 1.
- A set of vectors is said to be **orthogonal** if the inner product of each pair of the vectors from the set is 0.
- A set of vectors is said to be **orthonormal** if the set is orthogonal, and each vector has norm 1.

Adjoint

Let V be a FDIPS and let $\mathsf{T} \in \mathcal{L}(\mathrm{V})$. Then the **adjoint of** T is the operator $\mathsf{T}^* \in \mathcal{L}(\mathrm{V})$ such that

$$\langle \mathsf{T}(x), y \rangle = \langle x, \mathsf{T}^*(y) \rangle$$

The matrix representation of the adjoint of an operator is the adjoint of the matrix representation of the operator.

$$[\mathsf{T}^*]_\beta = [\mathsf{T}]_\beta{}^*$$

And adjoint of a matrix is the **conjugate-transpose** of the matrix.

Special operators

- **Normal operators**: $UU^* = U^*U$.
- **Unitary operators**: $UU^* = U^*U = I$. These are special cases of normal operators. Unitary operators preserve inner product in Hilbert space.
- **Self-adjoint operators**: $A^* = A$. These are the most important operators in quantum mechanics - these operators model the physical quantities. The **Hamiltonian** operator is self-adjoint too.
- **Orthogonal operators**: Loose definition is "unitary operators" of RVS.

Linear Algebra in Quantum Mechanics

- The vector space is a complex inner product space - **Hilbert space** $\mathcal{H}$.
- Different operators for different physical quantity. And each operator has an inherent "observable" value for all the "states" - states are the vectors of the Hilbert space.
- Dirac notation used for brevity and convenience.

Dirac notation

~~Until tomorrow.~~

Dirac Notation

- $|v\rangle$ denotes a Vector in an abstract complex vector space $\mathbb{V}$. Represents the state of a quantum system in Hilbert space. Represented using column vectors.
- $\langle f|$ denotes a linear functional $f : \mathbb{V} \to \mathbb{C}$. Mathematically written as $\langle f|v\rangle \in \mathbb{C}$. Represented using row vectors.

Eigenvalue Problem

Definition

Eigenvector If T is a linear transformation from a vector space V over a field $\mathbb{F}$ onto itself and v is a nonzero vector in V, then v is an eigenvector of T if $T(v)$ is a scalar multiple of v
$T(v) = \lambda v$

- Matrix representation:
  $Av = \lambda v$
- 3b1b intuition

Diagonalization

A square matrix A is called diagonalizable if there exists an invertible matrix P and a diagonal matrix D such that $P^{-1}AP = D$, or equivalently $PAP^{-1} = D$. (Such P, D are not unique.) For a finite-dimensional vector space V, a linear map $T : V \to V$ is called diagonalizable if there exists an ordered basis of V consisting of eigenvectors of T.
These definitions are equivalent: if T has a matrix representation $A = PDP^{-1}$ as above, then the column vectors of P form a basis consisting of eigenvectors of T, and the diagonal entries of D are the corresponding eigenvalues of T; with respect to this eigenvector basis, A is represented by D.
Diagonalization is the process of finding the above P and D.

Hermitian operators

- Self-adjoint: $\langle Av, w\rangle = \langle v, Aw\rangle$
- In a FDVS, equal to conjugate transpose
- Real eigenvalues
- Orthogonal eigenkets: $\langle n|m\rangle = \delta_{nm}$

Commutator

- What is commutation?
- As a measure of the extent to which a binary operation fails to commute
- Commutator: $[a, b] = ab - ba$
- Anticommutator: $\{a, b\} = ab + ba$

Postulates of Quantum Mechanics

Classical Mechanics
The state of a particle at any given time is specified by two variables $x(t)$ and $p(t)$, i.e., as a point in two-dimensional phase space

Quantum Mechanics
The state of the particle is described by a vector $|\Psi(t)\rangle$ in Hilbert space

Postulates of Quantum Mechanics (cont.)

Classical Mechanics

Every dynamical variable ω is a function of x and p: $\omega = \omega(x, p)$

Quantum Mechanics

The independent variables x and p of classical mechanics are expressed as operators X and P with the following matrix elements in the eigenbasis of X:

$$\langle x| X |x'\rangle = x\delta(x - x')$$
$$\langle x| P |x'\rangle = -i\hbar\delta'(x - x')$$

The operators corresponding to dependent variables $\omega = \omega(x, p)$ are given by Hermitian operators

$$\Omega(X, P) = \omega(x \to X, p \to P)$$

Postulates of Quantum Mechanics (cont.)

Classical Mechanics
If the particle is in a state given by x and p, the measurement of the variable ω will yield a value $\omega(x, p)$ and the state will remain unaffected

Quantum Mechanics
If the particle is in the state $|\Psi(t)\rangle$, measurement of the variable corresponding to Ω will yield one of the eigenvalues ω with the probability $P(\omega) \propto \|\langle\omega|\Psi\rangle\|^2$. The state of the system will change from $|\Psi\rangle$ to $|\omega\rangle$ on measurement

Postulates of Quantum Mechanics (cont.)

Classical Mechanics
The state variables change with time according to Hamilton's equations:

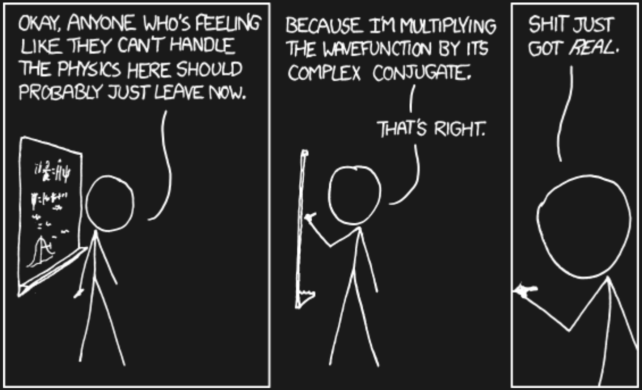
$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p} \qquad \dot{p} = -\frac{\partial \mathcal{H}}{\partial x}$$

Quantum Mechanics
The state vector ($|\Psi(t)\rangle$) obeys the Schrödinger Equation:

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

where $H(X, P) = \mathcal{H}(x \to X, p \to P)$ is the quantum Hamiltonian operator and $\mathcal{H}$ is the Hamiltonian for the corresponding classical problem.

Postulates of Quantum Mechanics (cont.)



Measurement

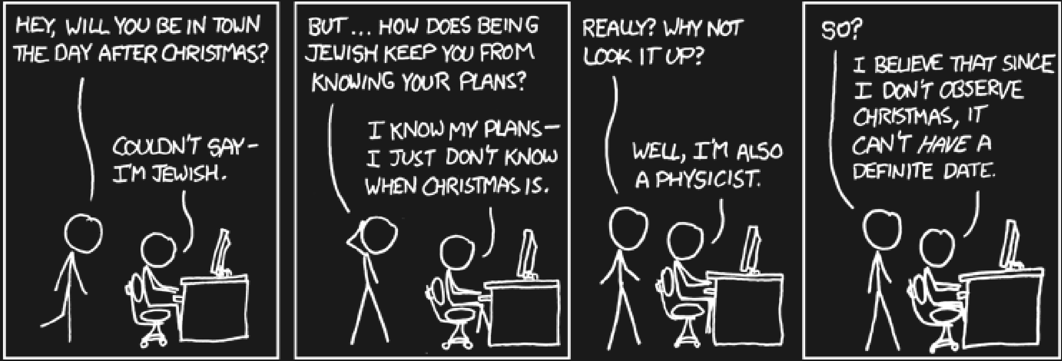
- In a certain eigenbasis, the state can thus be represented as:

$$|\Psi\rangle = \sum_i |\omega_i\rangle \langle\omega_i|\Psi\rangle$$

- Collapse of the wavefunction
- Probability of each eigenstate given by:

$$P(\omega_i) = \frac{\| \langle\omega_i|\Psi\rangle \|^2}{\langle\Psi|\Psi\rangle}$$

Collapse


HEY, WILL YOU BE IN TOWN THE DAY AFTER CHRISTMAS?
COULDN'T SAY - I'M JEWISH.
BUT... HOW DOES BEING JEWISH KEEP YOU FROM KNOWING YOUR PLANS?
I KNOW MY PLANS - I JUST DON'T KNOW WHEN CHRISTMAS IS.
REALLY? WHY NOT LOOK IT UP?
WELL, I'M ALSO A PHYSICIST.
SO?
I BELIEVE THAT SINCE I DON'T OBSERVE CHRISTMAS, IT CAN'T HAVE A DEFINITE DATE.

Expectation values

- Ensemble
- Expectation = mean value

$$\langle \Omega \rangle = \sum_i P(\omega_i)\omega_i$$
$$= \langle \Psi | \Omega | \Psi \rangle$$

- No need to solve IVP
- But if particle is in an eigenstate of Ω?

Uncertainty principle

- Standard deviation :

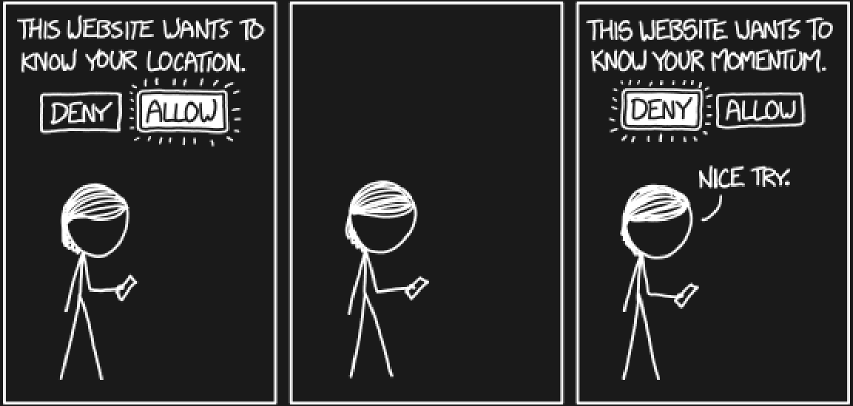
$$\Delta\Omega = \langle(\Omega - \langle\Omega\rangle)^2\rangle^{\frac{1}{2}}$$

- For position and momentum:

$$\Delta X.\Delta P \geq \frac{\hbar}{2}$$

- In operator algebra, $[X, P] = i\hbar$
- Operators that do not commute cannot be measured simultaneously and thus satisfy the uncertainty principle

Simultaneous measurement



Simultaneous diagonalization

- Operators that commute correspond to observables that can be measured simultaneously
- Operators O commuting with the Hamiltonian $\mathcal{H}$ are of special importance
- These observables correspond to constants of motion
- Thus, the system can be described by the Hilbert space spanned by that observable, i.e., $\mathcal{H}$ and O are simultaneously diagonalizable
- Mathematically, $\exists \; P$ such that $P^{-1}OP$ and $P^{-1}\mathcal{H}P$ are both diagonal matrices

Time dependent Schrödinger equation

The original equation that Schrödinger came up with, has a time-dependent Hamiltonian (due to a time-dependent potential)[2]:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \mathcal{H}\Psi(x,t) \tag{4}$$

If the potential is time-independent (and hence the Hamiltonian), we can use the separation of variables technique to simplify (4). Lets assume $\Psi(x,t) = \psi(x)\varphi(t)$. If we substitute this in (4), and separate terms according to the variable, we will get:

$$i\hbar\varphi(t)\frac{d\varphi(t)}{dt} = \frac{1}{\phi(x)}\mathcal{H}\psi(x) \tag{5}$$

[2] Only one dimensional equations will be considered for this session, but extension to higher dimension should not affect results.

Separation of Variables

Now both the sides have different variables, so for the equation to hold, both sides must equate to some constant, say E. From the right hand side then we have:

$$\mathcal{H}\psi(x) = E\psi(x) \tag{6}$$

Equation (6) is known as the **time independent Schrödinger equation**. And notice that this is an eigenvalue problem: E is the eigenvalue, and $\psi(x)$'s are the eigenvectors. In functional form, if you expand the expression for $\mathcal{H}$, we have

$$\left[\frac{1}{2m}\mathrm{P}^2 + V(x)\right]\psi(x) = E\psi(x) \tag{7}$$

The full wavefunction

The other equation (left hand side of (5)) yields the simple solution:

$$\varphi(t) = \mathrm{e}^{-iEt/\hbar} \tag{8}$$

Now we can recombine the two functions to get the solution for the wavefunction Ψ as $\Psi(x,t) = \mathrm{e}^{-iEt/\hbar}\psi(x)$ - this solution to the time independent Schrödinger equation is known as a *stationary state*, because the probability density of this wavefunction is constant in time:

$$\|\Psi(x,t)\|^2 = \Psi(x,t)^*\Psi(x,t) = \|\psi(x)\|^2 \tag{9}$$

Stationary state wavefunction of free particle

In the case of a free particle, the potential is $V(x) = 0$. From (7), we can get the solution to the spatial component as a linear combination of two *plane waves* - each travelling in opposite directions:

$$\psi_k(x) = a_1 \mathrm{e}^{ikx} + a_2 \mathrm{e}^{-ikx} \quad \left(k^2 = \frac{2mE}{\hbar^2}\right) \tag{10}$$

We will obtain the full wavefunction as:

$$\Psi_k(x,t) = a_1 \mathrm{e}^{ik\left(x - \frac{\hbar k}{2m} t\right)} + a_2 \mathrm{e}^{-ik\left(x + \frac{\hbar k}{2m} t\right)} \tag{11}$$

Issues with stationary state

Important points:

- Now the solution we obtained is a particular stationary state with energy corresponding to the value of k. If we consider the *de Broglie hypothesis*, and compare the velocity of the particle obtained from that and the velocity obtained from the expressions so far, the velocity of the quantum particle will be half the velocity of the classical particle.
- The wavefunction we derived is not normalizable, as the integral for normalisation diverges.

Superposition of stationary states

These two points entail to the fact that, stationary states of a free particle are not something which can be realised in the physical world. So comes to the rescue, **superposition** - the wavefunction exists as a linear combination of all possible stationary states. What this implies is that, the particle exists as a group of waves, or **wave packets**, the group velocity of which is the velocity of the particle.

Full solution for free particle

The full solution:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} c_k \mathrm{e}^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} dk \tag{12}$$

where the c_k are the normalisation coefficients, which can be calculated using

$$c_k = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) \mathrm{e}^{-ikx} dx \tag{13}$$

Infinite square well potential

In this case, we can define the potential to be:

$$V(x) = \begin{cases} 0 & , x \in [0, a] \\ \infty & , \text{otherwise} \end{cases} \tag{14}$$

Since the potential is infinite outside the well, the wavefunction of the particle in these regions is 0. While within the well, the solution for the wavefunction is same as that for a free particle (as $V = 0$).

Stationary state solution

The only addition in this problem is the boundaries - the existence of boundary at $x = 0$ and $x = a$ implies that the wavefunction has boundary condition restrictions, namely

$$\psi(0) = \psi(a) = 0$$

Applying the boundary condition, we can obtain the spatial part of the wavefunction as

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) \tag{15}$$

This is again, the spatial component of a single stationary state. The actual wave function will be a linear combination of all the stationary states, and will be normalised.

Full wavefunction for particle in well

The solution for actual wave function would be:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \mathrm{e}^{-i(n^2\pi^2\hbar/2ma^2)t} \tag{16}$$

The coefficients c_n can be calculated using

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0) dx \tag{17}$$

The End.