Introduction to Quantum mechanics and Linear Algebra

Physics Immersion Week Day 2
June 22, 2021

Main Quantum mechanics Concepts

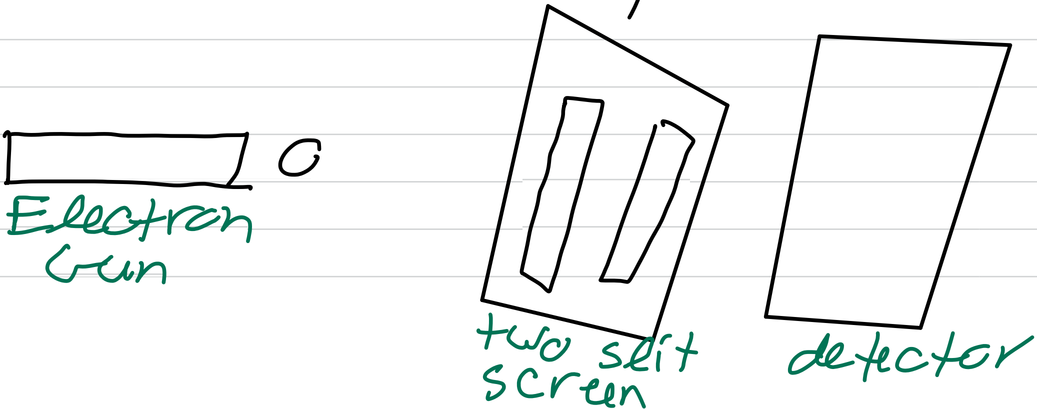
1. We need waves to describe particles
2. Some physical systems are quantized
3. Quantum systems have uncertainity

The Two Formulations of Quantum mechanics

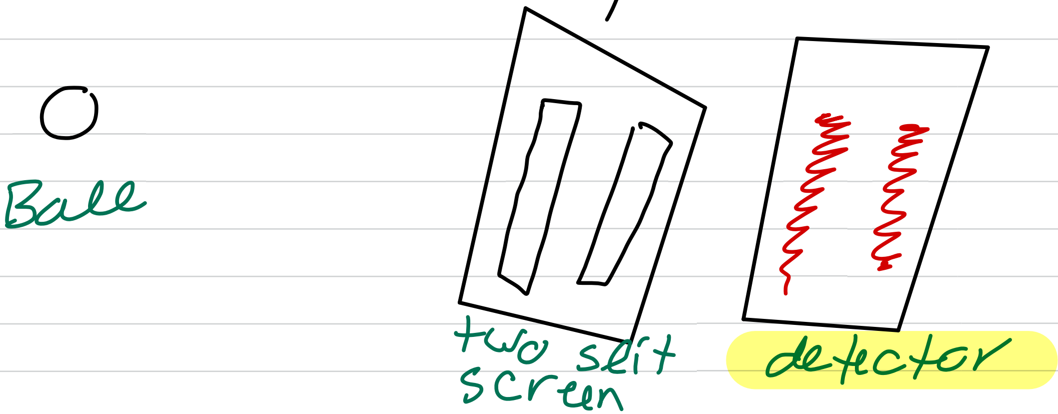
1. wave mechanics
2. matrix mechanics

The Breakdown of classical mechanics

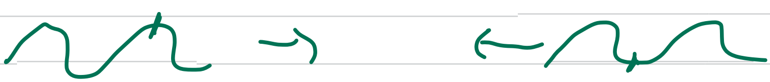
The Two-Slit Experiment



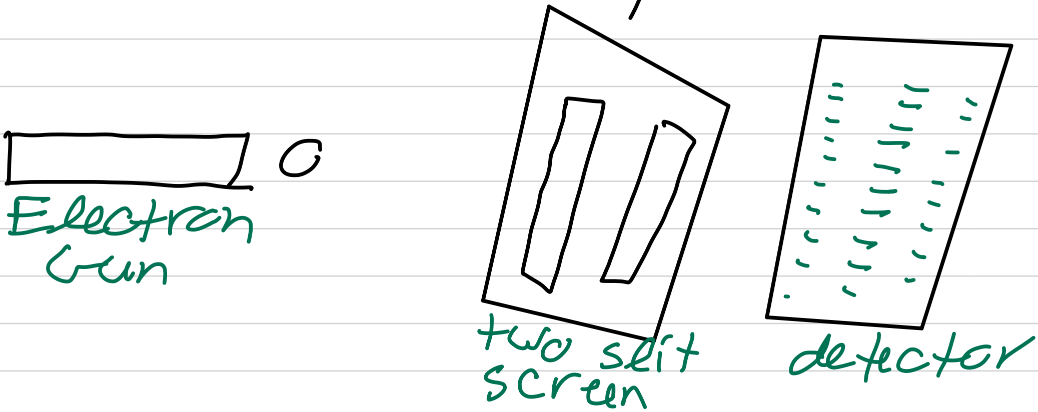
The Two-Slit Experiment



The Two-Slit Experiment



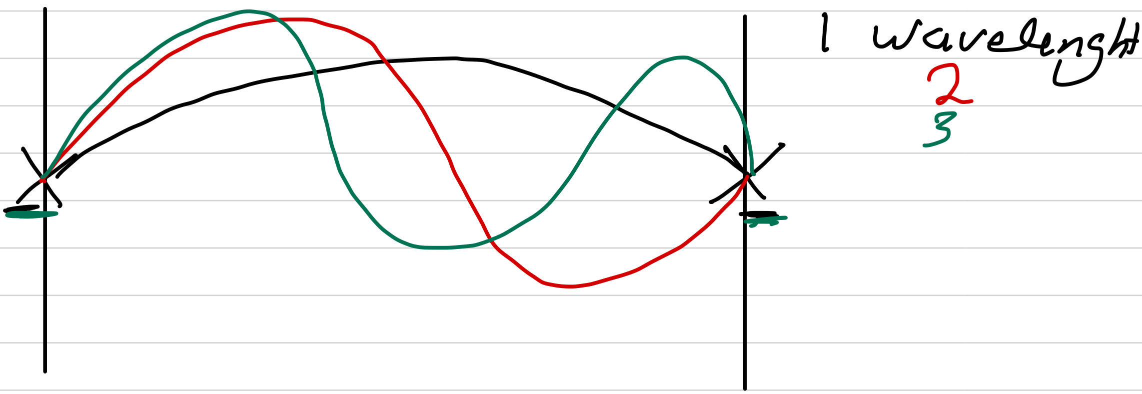
The Two-Slit Experiment



Wave particle Duality

- Electrons are particles but they can be described with wave equations

Quantized Values



Quantized Values

wavelength λ

Frequency $\nu = c/\lambda$

Energy $E = h\nu$

↳ Planck's constant

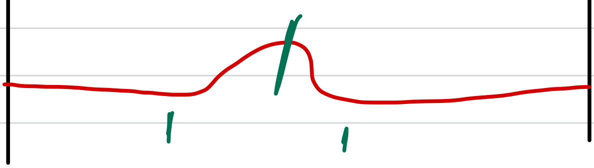
momentum $p = \sqrt{2mE}$

position - not quantized

Uncertainity

$\tilde{x}$, $\vec{p} \rightarrow m\vec{v}$

→ wave



→ wave

Complex Numbers

imaginary number $i = \sqrt{-1}$

$y = -x^2$

Property $\Rightarrow i^2 = -1$

Complex number

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

$Re(z) = a \qquad Im(z) = b$

Complex conjugate

$z = a + ib$

$z^* = a - ib$

Ex: $z = 2 - 3i + 4i$

$z^* = 2 + 3i - 4i$

$zz^* = |z|^2 = (a+ib)(a-ib)$

$= a^2 + b^2 \quad , \quad a, b \in \mathbb{R}$

Euler Identy: $e^{i\theta} = \cos\theta + i\sin\theta$

Matrices And Vectors

$$\vec{V} = \begin{bmatrix} V_0 \\ V_1 \\ V_2 \\ \vdots \\ V_N \end{bmatrix} \qquad A = \begin{bmatrix} a_{00} & a_{01} & \cdots & a_{0m} \\ a_{10} & a_{11} & \cdots & a_{1m} \\ a_{20} & a_{21} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n0} & a_{n1} & \cdots & a_{nm} \end{bmatrix}$$

vector matrix

Transpose:

$$\vec{V} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \Rightarrow \vec{V}^T = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}$$

column vector

row vector

$$\vec{X} = \begin{bmatrix} 4 & 5 & 6 \end{bmatrix} \Rightarrow \vec{X}^T = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

$$\Downarrow$$

$$A^T = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 5 & 9 \\ 2 & 6 & -1 \\ 3 & 7 & -2 \\ 4 & 8 & -3 \end{bmatrix} \qquad 4 \times 3$$

$$\Downarrow \text{ Transpose}$$

$$3 \times 4$$

$$\Downarrow$$

$$A^T = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & -1 & -2 & -3 \end{bmatrix}$$

Matrix/Matrix Multiplication

$$\left.\begin{array}{ll} A & m \times n \\ B & n \times p \end{array}\right]$$

$$AB = C \Rightarrow m \times p$$

Example

$A = [1 \quad 2 \quad 3]$ 1×3

$B = \begin{bmatrix} 4 & 5 \\ 6 & 7 \\ 8 & 9 \end{bmatrix}$ 3×2

$$AB = [1 \; 2 \; 3] \begin{bmatrix} 4 & 5 \\ 6 & 7 \\ 8 & 9 \end{bmatrix}$$

$$= [1(4) + 2(6) + 3(8) \quad 1(5) + 2(7) + 3(9)]$$

$$= [4 + 12 + 18 \quad 5 + 14 + 27]$$

$$= [34 \quad 46]$$

$$A = \begin{bmatrix} 2 & -1 \\ 1 & 3 \end{bmatrix}_{2\times 2} \qquad B = \begin{bmatrix} 4 & -1 \\ 1 & 2 \end{bmatrix}_{2\times 2}$$

$$AB =$$

$$\begin{bmatrix} 2 & -1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 4 & -1 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 2(4) + -1(1) & 2(-1) + -1(2) \\ 1(4) + 3(1) & 1(-1) + 2(3) \end{bmatrix}$$

$$= \begin{bmatrix} 8 - 1 & -2 - 2 \\ 4 + 3 & -1 + 6 \end{bmatrix}$$

$$= \begin{bmatrix} 7 & -4 \\ 7 & 5 \end{bmatrix}$$

Eigenvalues and Eigenvectors

$$\underset{n\times n}{A}\, \overset{\text{vector of length } n}{x} = \underset{\text{lambda, } \mathbb{R}, \mathbb{C}}{\lambda}\, x$$

x is an eigen vector of A
λ is an eigen value of A

$$Ax = \lambda x$$
$$Ax - \lambda x = 0$$
$$(A - \lambda I)x = 0 \Rightarrow \text{eigenvalues, eigenvector}$$

$$x^2 + x = 0 \Rightarrow \text{roots}$$

identity matrix : $I_{n\times n} = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots & \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ & \vdots & & & \end{bmatrix}$

Eigen value

A $n \times n$ determinant

$\rightarrow |A - \lambda I| = 0$

Example:

$$A = \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix}$$

$$\left| \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right| = 0$$

$$\left| \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \right| = 0$$

$$\begin{vmatrix} -\lambda & 1 \\ -2 & -3-\lambda \end{vmatrix} = 0$$

$$-\lambda(-3-\lambda) - 1(-2) = 0$$

$$3\lambda + \lambda^2 + 2 = 0$$

$$\lambda^2 + 3\lambda + 2 = 0$$

$$\lambda = \frac{-3 \pm \sqrt{9 - 4(1)(2)}}{2(1)}$$

$$= \frac{-3 \pm \sqrt{9-8}}{2} = \frac{-3 \pm 1}{2}$$

$$= -1, -2$$

Finding Eigenvector

$r_1 = -1$ $\qquad\qquad$ $r_2 = -2$

$$(A - rI)\vec{x} = \vec{0} \rightarrow \begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix}$$

$$\left(\begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix} + (+1) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) \vec{x} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\left(\begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\underset{2 \times 2}{\begin{bmatrix} 1 & 1 \\ -2 & -2 \end{bmatrix}} \underset{2 \times 1}{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}} = \underset{2 \times 1}{\begin{bmatrix} 0 \\ 0 \end{bmatrix}}$$

$$x_1 + x_2 = 0 \quad \Rightarrow \quad x_1 = -x_2$$

$$-2x_1 - 2x_2 = 0$$

$$\vec{x}_1 = \begin{bmatrix} 2 \\ -2 \end{bmatrix} \qquad\qquad x_1 = 2$$

$$x_2 = -2$$

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Wave Functions

$|\psi(x,t)\rangle$ – wave function
↳ ket → vector

$|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle$

Superposition principle

$\Rightarrow |\psi\rangle = a|\psi_1\rangle + b|\psi_2\rangle$ $\quad a,b \in \mathbb{C}, \mathbb{R}$

All possible wave function form a basis

spin of electron ↑ ↓

$|\psi_\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\psi_\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

$|\psi\rangle = a|\psi_\uparrow\rangle + b|\psi_\downarrow\rangle$

$= \begin{bmatrix} a \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ b \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$

$\vec{x} = (1 \quad 0 \quad 0)$
$\vec{y} = (0 \quad 1 \quad 0)$
$\hat{z} = (0 \quad 0 \quad 1)$

basis
length 3

$$\vec{r} = a\vec{x} + b\vec{y} + c\hat{z}$$

$$|\psi\rangle = a|\psi_1\rangle + |\psi_2\rangle$$

electron $\uparrow \quad \downarrow \quad \nearrow$

Born Interpretation $\rightarrow$ Statistics

Question: probabilities

$$|\psi\rangle = a|\psi_1\rangle + b|\psi_2\rangle$$

$$a, b \in \mathbb{C}$$

$$P_a + P_b = 1 \qquad |a|^2 + |b|^2 = 1$$

$$P(\psi; \psi_1) = |a|^2 = aa^* \in \mathbb{R}$$

$$P(\psi; \psi_2) = |b|^2 = bb^* \in \mathbb{R}$$

$$|\vec{v}| = \sqrt{v_1^2 + v_2^2 + v_3^2 + \cdots} = \sqrt{\underbrace{\vec{v}^T v}}$$

$|\psi\rangle$, transpose and complex conjugate

$$\underbrace{(|\psi\rangle^*)^T}_{\text{ket}} = \underbrace{\langle\psi|}_{\text{bra}}$$

$\langle\underbrace{\psi}|\underbrace{\psi}\rangle$ ~ Dirac notation
Bra(c)ket

$\langle\psi_1|\psi_2\rangle = 0$

$$\langle\psi|\psi\rangle = (\vec{v}^T)^* \vec{v}$$

$$|a|^2 + |b|^2 = 1 \Rightarrow \langle\psi|\psi\rangle = 1$$

$$|\psi\rangle = \overbrace{a|\psi_1\rangle} + b|\psi_2\rangle$$

$$\langle\psi|\psi\rangle = \langle\psi_1|a^*a|\psi_1\rangle + \langle\psi_2|b^*b|\psi_2\rangle$$

$$= a^*a \underbrace{\langle\psi_1|\psi_1\rangle}_{1} + b^*b \underbrace{\langle\psi_2|\psi_2\rangle}_{1}$$

$$= \underbrace{|a|^2 + |b^2|} = 1$$

to normalize a wavefunction

$$|\psi\rangle_N = \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}}$$

$\langle\psi|\psi\rangle \rightarrow$ dot product

$\hookrightarrow$ inner product

$$|\psi\rangle = \begin{bmatrix} i \\ 3 \\ 2+3i \end{bmatrix} \rightarrow \text{ket}$$

$$\langle\psi| = \begin{bmatrix} -i & 3 & 2-3i \end{bmatrix}$$

$$\underbrace{\langle\psi|\psi\rangle}_{} = \underset{1\times 3}{\begin{bmatrix} -i & 3 & 2-3i \end{bmatrix}} \begin{bmatrix} i \\ 3 \\ 2+3i \end{bmatrix}_{3\times 1}$$

$$= [-i(i) + (3)3 + (2-3i)(2+3i)]$$

Quantum Basics wrap-up
Operators and Expectation Values

Wavefunction: (Superposition principle)

$|\psi\rangle = a|\psi_1\rangle + b|\psi_2\rangle$

$|\psi\rangle \rightarrow$ vector

$|\psi_2\rangle \rightarrow$ basis vectors

dot/inner product (vector-vector multiplication)

$\langle\psi|\psi\rangle = |a|^2 + |b|^2$

$\langle\psi_1|\psi_1\rangle = 1$

$\langle\psi_2|\psi_2\rangle = 1$

$\langle\psi_1|\psi_2\rangle = 0$

$\langle\psi_2|\psi_1\rangle = 0$

Operator → matrices

momentum → $\hat{p}$

$\hat{p}|\psi\rangle = p|\psi\rangle$

$p \rightarrow$ momentum

eigenvalue / eigenvector

operator → Hermitian

↓

real eigenvalues

Hamiltonian - operator that gives energy

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

Expectation value

$$|\psi\rangle = a|\psi_1\rangle + b|\psi_2\rangle$$

$|a|^2$ $|b|^2$

$$R|\psi_1\rangle = p_1|\psi_1\rangle$$
$$R|\psi_2\rangle = p_2|\psi_2\rangle$$

$$\underset{\text{ket}}{R|\psi\rangle} = a p_1|\psi_1\rangle + b p_2|\psi_2\rangle$$

$$\langle\psi|\underset{\text{expectation value}}{R}|\psi\rangle = \langle\psi_1|a^* p_1 a|\psi_1\rangle + \langle\psi_2|b^* p_2 b|\psi_2\rangle$$
$$= \underline{a^* p_1 a}\, \cancel{\langle\psi_1|\psi_1\rangle} \rightarrow 1$$
$$+ b^* p_2 b\, \cancel{\langle\psi_2|\psi_2\rangle} \rightarrow 1$$
$$= a^* a\, p_1 + b^* b\, p_2$$
$$= \underset{\text{probability}}{|a|^2}\, p_1 + |b|^2\, p_2$$

average = 0.5 (heads) + 0.5 (tails)