Contents

1. Schrödinger Equation

Quantum state of an object is defined by "wave function": $\psi(\vec{x}, t)$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + v(\vec{x})\psi = i\ \hbar\ \frac{\partial\psi}{\partial t}$$

2. Postulates of QM

1. The state of a QM system is completely specified by the wave function, $\psi(\vec{x}, t)$. ψ has the property that

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \psi^* \psi = 1$$

2. To every observable in QM, there is a corresponding Hermitian operator:

Observable	Operator	Operation
x	$\hat{x}$	$x \cdot \psi(x, t)$
p	p	$-i\ \hbar \cdot \frac{\partial}{\partial x}\psi(x, t)$
E	$\hat{H}$	$\left[\frac{1}{2m}\hat{p}^2 + V(x)\right]\psi$
$V(x)$	$\hat{V}(x)$	$V(x)\psi$

3. Any measurement of the observable $\hat{A}$, we only ever observe the eigenvalues, a, that satisfy

$$\hat{A}\psi = a\psi$$

The values of dynamical variables are quantized.

4. If the system is in a state described by ψ, then the average/expected value of the observable corresponding to $\hat{A}$ is:

$$\langle A \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^* \hat{A} \psi$$

5. The wave function evolves in time according to the time-dependent Schrödinger Equation:

$$\hat{H}\psi = i\ \hbar\ \frac{\partial \psi}{\partial t} \left(i\ \hbar\ \frac{\partial}{\partial t} \sim E\right)$$

6. Pauli Exclusion Principle: electrons can't occupy the same space

3. Deriving Schrödinger Equation of One Dimension

The electric field must obey wave equation:

$$E(x, t) = E_0 e^{i(kx - \omega t)} \text{ satisfy } \frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2}$$

Since:

$$\frac{\partial^2 E}{\partial x^2} = -E_0 k^2 e^{i(kx-\omega t)} \text{ and } \frac{\partial^2 E}{\partial t^2} = -E_0 \omega^2 e^{i(kx-\omega t)}$$

The relationship between k and ω is:

$$k^2 = \frac{\omega^2}{c^2}$$

Given:

$$E = \hbar\ \omega \text{ and } p = \hbar\ k$$

By substitution, we have:

$$E = E_0 e^{\frac{i}{\hbar}(px-Et)}$$

Applying the wave equation, we get:

$$\begin{aligned}
\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)E &= 0 \\
-E_0 \frac{p^2}{\hbar^2} e^{\frac{i}{\hbar}(px-Et)} + E_0 \frac{E^2}{\hbar^2 c^2} e^{\frac{i}{\hbar}(px-Et)} &= 0 \\
-\frac{E_0}{\hbar^2} e^{\frac{i}{\hbar}(px-Et)} \left(\frac{E^2}{c^2} - p^2\right) &= 0 \\
\frac{E^2}{c^2} - p^2 &= 0 \\
E^2 &= p^2 c^2
\end{aligned}$$

When modify wave equation to account for massive, relativistic objects, we have Klein-Gordon equation:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2 c^2}{\hbar^2}\right)\psi = 0$$

Plugging in electric field and swap $E \to \psi$:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\left(\psi_0 e^{\frac{i}{\hbar}(px-Et)}\right) = 0$$

$$-\frac{p^2}{\hbar^2}\psi + \frac{E^2}{\hbar^2c^2}\psi - \frac{m^2c^2}{\hbar^2}\psi = 0$$

$$p^2c^2 + m^2c^4 = E^2$$

which is the relativistic energy-momentum relation.

Consider the non-relativistic limit $p^2 \ll m^2c^2$:

$$\begin{aligned}
\psi &= \psi_0 \exp\left(\frac{i}{\hbar}\left[px - (p^2c^2 + m^2c^4)^{\frac{1}{2}}t\right]\right) \\
&= \psi_0 \exp\left(\frac{i}{\hbar}\left[px - mc^2\left(\frac{p^2c^2}{m^2c^4} + 1\right)^{\frac{1}{2}}t\right]\right) \\
&\approx \psi_0 \exp\left(\frac{i}{\hbar}\left[px - mc^2\left(\frac{1}{2}\frac{p^2c^2}{m^2c^4} + 1\right)t\right]\right) \text{ using } (1+x)^n \approx 1 + nx \\
&= \psi_0 \exp\left(\frac{i}{\hbar}\left[px - \left(\frac{p^2}{2m} + mc^2\right)t\right]\right) \\
&= \psi_0 \exp\left(-\frac{i}{\hbar}mc^2t\right)\exp\left(\frac{i}{\hbar}(px - \mathcal{T}t)\right) \\
&\text{where } \mathcal{T} = \frac{p^2}{2m} \text{ (classical kinetic energy)}
\end{aligned}$$

$$\psi = \psi_0 \exp\left(-\frac{i}{\hbar}mc^2t\right)\varphi$$

$$\text{where } \varphi = \exp\left(\frac{i}{\hbar}(px - \mathcal{T}t)\right)$$

$$\begin{aligned}
\frac{\partial^2 \psi}{\partial t^2} &= \frac{\partial}{\partial t}\frac{\partial \psi}{\partial t} \\
&= \frac{\partial}{\partial t}\left(-\frac{i}{\hbar}mc^2 \exp\left(-\frac{i}{\hbar}mc^2 t\right)\varphi + \exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial \varphi}{\partial t}\right) \\
&= -\frac{m^2c^4}{\hbar^2}\exp\left(-\frac{i}{\hbar}mc^2 t\right)\varphi - \frac{2i}{\hbar}mc^2 \exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial \varphi}{\partial t} \\
&\quad + \exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial^2 \varphi}{\partial t^2}
\end{aligned}$$

Plugging into the Klein-Gordon equation:

$$\begin{aligned}
\frac{\partial^2 \psi}{\partial x^2} + \frac{m^2c^2}{\hbar^2}\exp\left(-\frac{i}{\hbar}mc^2 t\right)\varphi + \frac{2i}{h}m\exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial \varphi}{\partial t} \\
-\frac{1}{c^2}\exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial^2 \varphi}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\exp\left(-\frac{i}{\hbar}mc^2 t\right)\varphi = 0 \\
\frac{\partial^2 \psi}{\partial x^2} + \frac{2i}{\hbar}m\exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial \varphi}{\partial t} - \frac{1}{c^2}\exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial^2 \varphi}{\partial t^2} = 0
\end{aligned}$$

Since the term with c^{-n} is really small, we have:

$$\begin{aligned}
\exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial^2 \varphi}{\partial x^2} + \frac{2i}{\hbar}m\exp\left(-\frac{i}{\hbar}mc^2 t\right)\frac{\partial \varphi}{\partial t} = 0 \\
\frac{\partial^2 \varphi}{\partial x^2} = -\frac{2mi}{\hbar}\frac{\partial \varphi}{\partial t} \\
-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} = i\ \hbar\ \frac{\partial \varphi}{\partial t}
\end{aligned}$$

which is Schrödinger equation of one dimension.

4. Probability

$$\int_a^b \mathrm{d}x\, |\psi(x,t)|^2 = \text{prob. of finding the particles in } [a,b]$$

5. Where was the particle before we measure it?

1. Realist position: position was near c (Einstein's position)
   - QM is incomplete
2. Orthodox position / Copenhagen Interpretation - particle was not anywhere (Bohr, most popular among physicists)
   - something peculiar about "measurement"
3. Agnostic position - dismiss the question as metaphysics

1960s: John Bell shows there's an experimental difference between the realist and orthodox position

- Bell's Theorem
- Orthodox position is experimentally confirmed

6. Normalization

ψ is a solution to the Schrödinger equation.

$A\psi$ will also be a solution, where $A \in \mathbb{C}$

Normalization is the process of fixing A to have definite value:

$$|A|^2 \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^* \psi = 1$$

7. Momentum Operator

$$\langle x\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^* x \psi$$

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \int_{-\infty}^{\infty} \mathrm{d}x\, \frac{\partial}{\partial t}(x\psi^*\psi) \quad = \frac{i\ \hbar}{m}\int_{-\infty}^{\infty} \mathrm{d}x\, x\frac{\partial}{\partial t}\left(\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x} + \psi\frac{\mathrm{d}\psi^*}{\mathrm{d}x}\right)$$

$$\langle v\rangle = -\frac{i\ \hbar}{m}\int_{-\infty}^{\infty} \mathrm{d}x\, \psi^* \frac{\partial}{\partial x}\psi$$

$$\langle p\rangle = -i\ \hbar \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^* \frac{\partial}{\partial x}\psi$$

If we can measure 2 observable at the same time meaning 1 does not impact our ability to measure the other — "compatible" observables

7.1. Commutator of 2 Ops

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} = \begin{cases} = 0 \text{ obs. are compatible} \\ \neq 0 \text{ obs. are incompatible} \end{cases}$$

8. Canonical Commutation Relation

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\ \hbar$$

$$[\hat{x}, \hat{x}^n] = 0, [\hat{p}, \hat{p}^n] = 0, [E, t] \neq 0$$

9. Heisenberg Uncertainty Principle

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

9.1. Generalized Uncertainty Principle

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

10. The Time Independent Schrödinger Equation

We find $\Psi(\vec{x}, t)$ by specifying a potential of $V(\vec{x})$ by solving the Schrödinger Equation:

How do we solve PDEs? Separation of variables.

$$\Psi(x, t) = \psi(x, t) \cdot \varphi(t)$$

$$\frac{\partial \Psi}{\partial t} = \psi(x) \frac{\mathrm{d}\varphi}{\mathrm{d}t} \quad \frac{\partial^2 \Psi}{\partial x^2} = \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} \cdot \varphi(t)$$

Substituting into the Schrödinger Equation:

$$-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} \psi + V(x) \psi \varphi = i\ \hbar\ \psi \frac{\mathrm{d}\varphi}{\mathrm{d}t}$$
$$-\frac{\hbar^2}{2m} \cdot \frac{1}{\psi} + V(x) = i\ \hbar\ \frac{1}{\psi} \frac{\mathrm{d}\varphi}{\mathrm{d}t}$$

Can only be true if both sides are equal to a constant E:

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \cdot \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} + V(x) = E$$

$$\boxed{-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} + V(x) \psi(x) = E \psi(x)}$$

which is the time-independent Schrödinger equation.

$$i\ \hbar\ \frac{\mathrm{d}\varphi}{\mathrm{d}t} = E \varphi(t) \quad \text{since } \frac{1}{i} = -i$$
$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -i \frac{E}{\hbar} \varphi(t) \to \varphi(t) = \exp\left(-iE \frac{t}{\hbar}\right)$$

General solutions to S.E take the form:

$$\Psi(x, t) = \psi(x) \exp\left(-iE \frac{t}{\hbar}\right)$$

1. Separable solutions are "stationary states"

$$|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) = |\psi(x)|^2$$

$$\begin{aligned}\left\langle \hat{Q}(x,p) \right\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x\, \Psi^*(x,t)\hat{Q}\left(x, \frac{\partial}{\partial x}\right)\Psi(x,t) \\ &= \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^*(x)\hat{Q}\psi(x)\end{aligned}$$

2. These are states of definite energy
   in Q.M., the total energy is given by the "Hamiltonian": $H = \frac{p^2}{2m} + V(x)$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \to \hat{H}\psi(x) = E\psi(x)$$

$$\begin{aligned}\left\langle \hat{H} \right\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^*(x)\left(\hat{H}\psi(x)\right) \\ &= E\int_{-\infty}^{\infty} \mathrm{d}x\, \psi^*(x)\psi(x) = E \\ \left\langle \hat{H}^2 \right\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^*(x)\left[\hat{H}\left(\hat{H}\psi(x)\right)\right] = E^2 \\ \sigma_{\hat{H}}^2 &= \left\langle \hat{H}^2 \right\rangle - \left\langle \hat{H} \right\rangle^2 = 0\end{aligned}$$

3. We'll find that T.I.S.E permits an ∞ number of solutions, each with a different energy E_n.
   We can write the general solutions to the S.E for any potential V(x) as the "superposition" / linear combination of separable states.

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp\left(-iE_n \frac{t}{\hbar}\right)$$

We'll find that the coefficients c_n by looking at the boundary conditions.

11. Infinite Square Well

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

T.I.S.E:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = E\psi$$

In the well:

$$-\frac{\hbar}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi$$

Take $k := \frac{\sqrt{2mE}}{\hbar}$, we have:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -k^2\psi \Rightarrow \psi(x) = A\sin(kx) + B\cos(kx)$$

Boundary conditions:

1. ψ is continuous
2. $\frac{\mathrm{d}\psi}{\mathrm{d}x}$ is continuous

$$\psi(x=0) = A\sin(0) + B\cos(0) = 0 \Rightarrow B = 0$$

$$\psi(x=a) = A\sin(ka) \Rightarrow \sin(ka)$$

Distinct solutions:

$$k_n = \frac{n\pi}{a}, n \in \mathbb{N} \Rightarrow k_n^2 = \frac{2mE_n}{\hbar}$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

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

$n = 1$: "ground state"
$n \neq 1$: "excited states"

11.1. Important properties of $\{\psi_n(x)\}$

1. They're mutually orthogonal

$$\int_0^a \mathrm{d}x\, \psi_n^*(x)\psi_m(x) = \begin{cases} 0 & \text{if } n \neq m \\ 1 & \text{if } n = m \end{cases}$$

2. They're "complete":

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right)$$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp\left(-\frac{iE_n t}{\hbar}\right)$$

$$\int \mathrm{d}x\, \psi_m^*(x)\Psi(x,0) = \sum_{n=1}^{\infty} c_n \int \mathrm{d}x\, \psi_m^*(x)\psi_n(x) = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$

$$\text{where } \delta_{mn} = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}$$

For the infinite square well:

$$\Psi(x,t) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right) \exp\left(-\frac{in^2\pi^2\ \hbar\ t}{2ma^2}\right)$$

$$c_n = \int \mathrm{d}x\, \psi_n^*(x)\Psi(x,0)$$

11.2. Interpretation of c_n

$$|c_n|^2 = \text{probability that a measurement of the energy yields } E_n$$

1. $$\sum_{n=1}^{\infty} |c_n|^2 = 1$$

2. $$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n \quad \text{(expectation value of the energy)}$$