The Quantum World

A Rapid Introduction: Day 2

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Recap

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- **Matter Waves**: classical dynamical variables $\rightarrow$ quantum wave function ('carrier' of probabilistic information).
- **Observables**: physical measurables (energy, position, momentum, etc...) are promoted to operators.
- **Schrödinger's Equation**: the governing equation for all of quantum mechanics.

Overview

Building Tools for Measurement: Commutators

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- This structure is called the **commutator** (a.k.a the bracket) and is defined as follows:

Definition

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$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{1}$$

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- These commutators satisfy some very useful properties (see next slide).

Building Tools for Measurement: Commutators

Here is a list of **commutator properties**:

- $\left[\hat{A}, \hat{A}\right] = 0$
- $\left[\hat{A}, \hat{B}\right] = -\left[\hat{B}, \hat{A}\right]$
- $\left[\hat{A}, \hat{B} \pm \hat{C}\right] = \left[\hat{A}, \hat{B}\right] \pm \left[\hat{A}, \hat{C}\right]$
- $\left[\hat{A}\hat{B}, \hat{C}\right] = \hat{A}\left[\hat{B}, \hat{C}\right] + \left[\hat{A}, \hat{C}\right]\hat{B}$
- $\left[\hat{A}, \hat{B}\hat{C}\right] = \hat{B}\left[\hat{A}, \hat{C}\right] + \left[\hat{A}, \hat{B}\right]\hat{C}$
- $\left[\hat{A}, \left[\hat{B}, \hat{C}\right]\right] + \left[\hat{C}, \left[\hat{A}, \hat{B}\right]\right] + \left[\hat{B}, \left[\hat{C}, \hat{A}\right]\right] = 0$

Quantum Promotions: Activity 2

Compute the commutator between $\hat{x}$ and $\hat{p}$, $[\hat{x}, \hat{p}]$.

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Compute the commutator between $\hat{x}$ and $\hat{p}$, $[\hat{x}, \hat{p}]$.
(*Hint: try applying the commutator to some arbitrary test function* $\psi(x)$.)

Building Tools for Measurement: Inner Products

- When working in the continuous function space, we can define an inner product as follows:

Definition

For 2 continuous, complex functions $f(x)$ and $g(x)$, the **inner product** *of $f(x)$ with $g(x)$ is defined as,*

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- This allows us to look for the 'overlap' between 2 wave functions.
- by the normalization condition, we have that:

$$0 \leq |\langle \psi, \phi \rangle| \leq 1$$

Building Tools for Measurement: Expectation

- The expectation value of an observable gives us a weighted average of all its possible values upon *measurement*.

Definition

Given an operator $\hat{Q}$ *and an arbitrary quantum state* Ψ*, the* **expectation value** *of that operator on* Ψ *is defined as*

$$\langle \hat{Q} \rangle_{\Psi} = \langle \Psi, \hat{Q}\Psi \rangle = \int_{-\infty}^{+\infty} dx \left(\Psi^* \hat{Q} \Psi \right) \tag{2}$$

Building Tools for Measurement: Uncertainty

- From the non-vanishing commutator between quantum observables, this causes uncertainty between the measuring of conjugate variables.

Heisenberg Uncertainty Principle

Given 2 observables $\hat{A}$ and $\hat{B}$ that do **not** *commute, there will be an uncertainty relation when measuring the 2 observables on a quantum state ψ given by*

$$\sigma_{\hat{A}}^2 \sigma_{\hat{B}}^2 \geq \left| \frac{1}{2i} \langle \psi, \left[\hat{A}, \hat{B} \right] \psi \rangle \right|^2$$

where σ is the uncertainty of an observable defined by $\sigma_{\hat{A}} = \sqrt{\langle \hat{A}^2 \rangle_\psi - \langle \hat{A} \rangle_\psi^2}$.

Building Tools for Measurement: Spectral Theorem

- **Hermiticity** is a property of all observables and ensures that their associated measured values are guaranteed to be **real**.

Definition

Given an operator A acting on a Hilbert space $\mathcal{H}$, the operator is said to be **Hermitian** *if*

$$\langle \Psi, A\Psi \rangle = \langle A\Psi, \Psi \rangle$$

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- Knowing this, we look at 2 theorems which together, constitute the **spectral theorem** and is key to our understanding of measurement in QM.

Building Tools for Measurement: Spectral Theorem

- First, we look at the notion of diagonalization:

Theorem

A linear operator Q on a Hilbert space $\mathcal{H}$ is **diagonalizable** *iff there exists an ordered set of eigenstates $\{\psi_i\}$ with corresponding eigenvalues $\{\alpha_i\}$ such that these eigenstates* **span** *the Hilbert space.*

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Theorem

The eigenstates of a Hermitian operator form an orthogonal set of states. (This is in fact an orthogonal basis that spans the observables' state space.)

Building Tools for Measurement: Activity 1

Prove the 2 theorems in the previous slide.
(*Hint: Recall the definition of Eigenvalues, Eigenvectors and Hermitian operators.*)

Building Tools for Measurement: Measurement

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Measurement Postulate

Given a diagonalizable Hermitian observable $\hat{Q}$ and an arbitrary quantum state expressed as the superposition of $\hat{Q}$ eigenstates $\Psi = \sum_j \alpha_j \psi_j$, performing a measurement of $\hat{Q}$ on Ψ would cause it to collapse into one of the eigenstates ψ_j with probability $|\alpha_j|^2$. The measurement outcome would be the eigenvalue q_j associated to ψ_j.

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- We will now explore a specific kind of energy eigenstate known as **stationary states**.

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- Plugging these into the Schrödinger equation, we get:

$$i\hbar\frac{df(t)}{dt} = Ef(t), \quad \hat{H}\psi(x) = E\psi(x)$$

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- Recall that any arbitrary quantum state can be constructed from a superposition of eigenstates (spectral theorem). Hence any quantum state can be written as:

$$\Psi(x,t) = \sum_{n=1}^{\infty} \alpha_n \Psi_n(x,t) = \sum_{n=1}^{\infty} \alpha_n \psi_n(x) e^{-\frac{iE_n}{\hbar}t}$$

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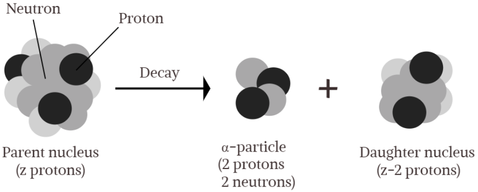

Figure: α-Particle Decay

What Now Schrödinger?: Ionization Smoke Detectors

Ionization is actually utilized in a common household appliance, smoke detectors.

Figure: Ionization Smoke Detector

The approximate model for the radial potential can be visualized as follows.

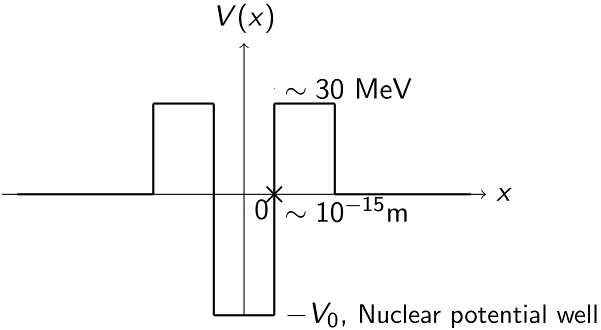

Figure: Simplified Radial Potential (not to scale)

What Now Schrödinger?: In the Nuclear Well

- In the region $x \in [-R, R]$, the Schrödinger equation is:

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  where k is known as the *wave number*.
- The solution to this ODE is:

$$\psi(-R < x < R) = Ae^{ikx} + Be^{-ikx} \tag{4}$$

  where A and B are complex coefficients to be solved via boundary conditions.

What Now Schrödinger?: In the Nuclear Well

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- This implies a **quantization** of the momentum and energy!

$$p_n = \frac{(2n-1)\pi\hbar}{2R}, \quad E_n = \frac{\hbar^2(2n-1)^2\pi^2}{8mR^2}$$

What Now Schrödinger?: Activity 1

Find the explicit wave function solutions to the infinite square well (nuclear well) potential.
(*Hint: Make use of the ansatz already previously provided.*)

What Now Schrödinger?: In the Nuclear Well

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Theorem

For a 1D bound state, the number of nodes increases linearly with the 'quantization index' n following the relation

$$\textit{number of nodes} = (n-1), \quad \textit{for} \;\; n = 1, 2, 3...$$

What Now Schrödinger?: Classically Forbidden Regions

- For the $x \in [R, R_c]$ and $x \in [-R_c, -R]$ regions, the energy of the α-particle is lower than the strength of the nuclear potential barrier V_n. The Schrödinger equation is:

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- We get the following solution:

$$\psi(R < x < R_c) = Ce^{-\kappa x}$$

where we ignore the exponentially growing solution.

- Lastly, we look at the region $x \in [R_c, \infty)$. Here, we have a free-particle Schrödinger's equation:

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What Now Schrödinger?: Freed from Nuclear Entrapment

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- The solution is thus:

$$\psi(x > R_c) = Ee^{ik'x}$$

where the wave number is $k'^2 \equiv \frac{2mE_\alpha}{\hbar^2}$ and $E_\alpha > 0$.

Joining the 3 solutions for the 3 separate regions:

$$\psi(x) = \begin{cases} Ee^{-ik'x}, & -\infty < x < -R_c \\ Ce^{\kappa x}, & -R_c < x < -R \\ Ae^{ikx} + Be^{-ikx}, & -R < x < +R \\ Ce^{-\kappa x}, & +R < x < +R_c \\ Ee^{-ik'x}, & +R_c < x < +\infty \end{cases}$$

(Visualization shown on the next slides.)

What Now Schrödinger?: Joining the Puzzle Pieces

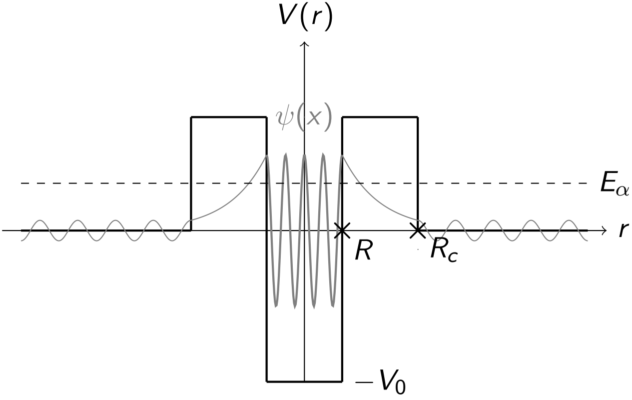

Figure: Visualization of the Wave Function

Break

Overview

1. Building Tools for Measurement
2. What Now Schrödinger?
3. Dirac's Bras and Kets

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- How do we resolve these 2 seemingly unrelated mathematical objects?
- Firstly we have to be clear about what caused us to use these difference different objects.
- **Finite (discrete) state space** vs **infinite (contiuous) state space**.

Dirac's Bras and Kets: Matrix Mechanics

- In Mach-Zehnder interferometry, states were confined to 2 possible configurations $\{|u\rangle, |d\rangle\}$ $\Rightarrow$ no need to provide a representation with any more than 2 complex numbers.

Dirac's Bras and Kets: Matrix Mechanics

- In Mach-Zehnder interferometry, states were confined to 2 possible configurations $\{|u\rangle, |d\rangle\}$ $\Rightarrow$ no need to provide a representation with any more than 2 complex numbers.
- The wave function formalism requires mathematical objects to be labelled by a continuous variable x (position). But it is theoretically possible to have a (infinitely long) vector analog known as a '**ket**'.

$$\psi(x) \to |\psi\rangle = \begin{bmatrix} \vdots \\ \psi(-2\epsilon) \\ \psi(-\epsilon) \\ \psi(0) \\ \psi(+\epsilon) \\ \psi(+2\epsilon) \\ \vdots \end{bmatrix}$$

Thank you!

https://tinyurl.com/TQWday2