

Lecture 8

Operators, States, and Basis in Quantum Mechanics

In this lecture you will learn:

- How to formulate a basis-independent way of doing quantum physics
- Representation of observables as operators
- Representation of quantum states as vectors

The Quantum Story Continues: Inductive Reasoning

Some fundamental universal principle (??)

Wavefunction

$$\psi(\vec{r}, t)$$

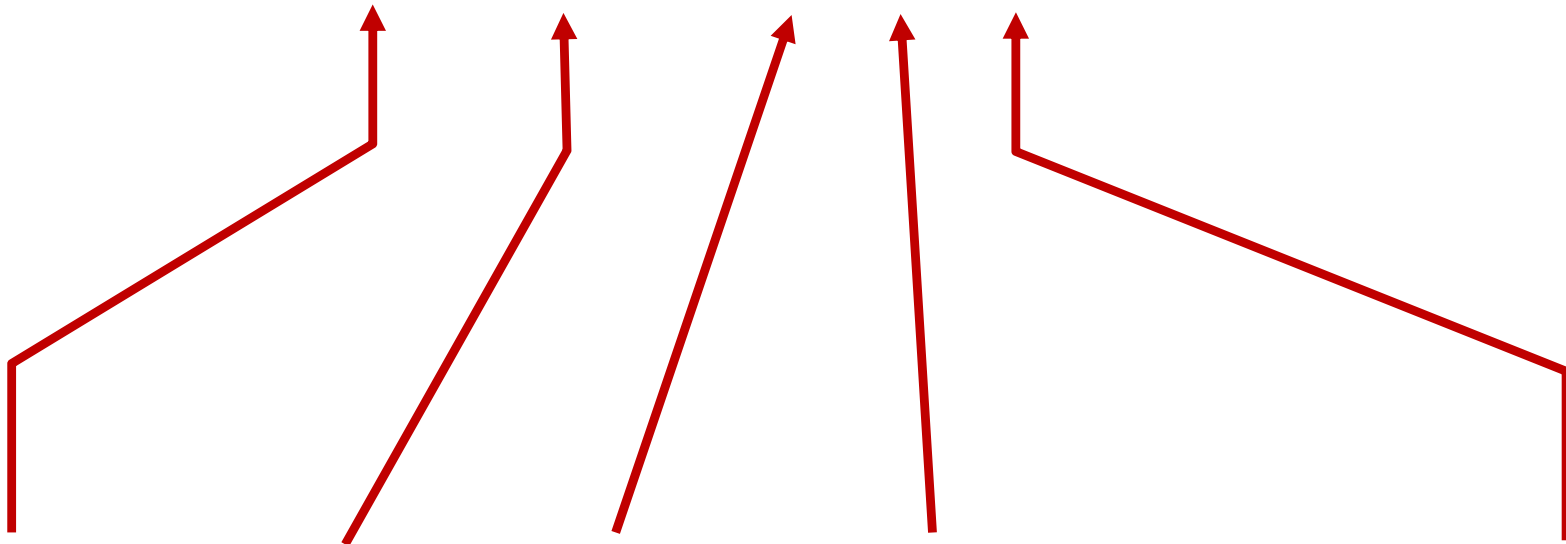
Spin



Light and photons

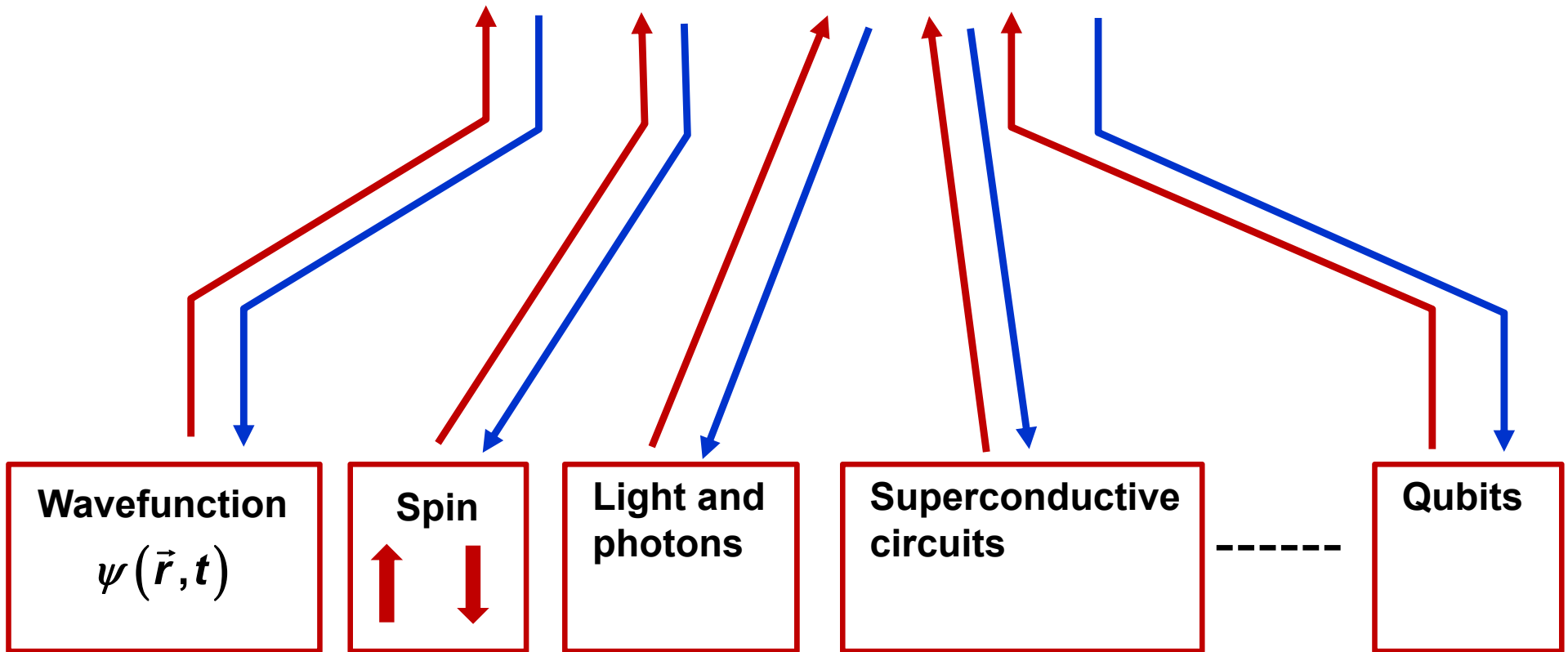
Superconductive circuits

Qubits



The Quantum Story Continues: Deduction

Some fundamental universal principle (??)



The Fundamental Principle: The Quantum State

A quantum state (of any particle or system) is represented by the state vector $|\psi(t)\rangle$ which is a vector in a Hilbert space

Quantum State vs Quantum Wavefunction of a Particle

A quantum state of a particle is fully described by the state vector $|\psi(t)\rangle$

The quantum state $|\psi(t)\rangle$ is the real deal !

We can write the **projection** of the vector $|\psi(t)\rangle$ or the component of the vector $|\psi(t)\rangle$ in position basis as:

$$\underbrace{\psi(x, t)} = \langle x | \psi(t) \rangle$$

We call it the “wavefunction” !

The wavefunction $\psi(x, t)$ is a “component” of the state vector in the position basis

$$|\psi(t)\rangle = \hat{1} |\psi(t)\rangle = \left(\int_{-\infty}^{\infty} dx |x\rangle \langle x| \right) |\psi(t)\rangle = \int_{-\infty}^{\infty} dx |x\rangle \langle x | \psi(t) \rangle = \int_{-\infty}^{\infty} dx \psi(x, t) |x\rangle$$

Complete Basis Sets in 1D

So far we have seen the following complete basis sets for the Hilbert space of square integrable functions in 1D:

Position basis:
$$\int_{-\infty}^{\infty} dx |x\rangle\langle x| = \hat{1}$$

Orthogonality:
$$\langle x' | x \rangle = \delta(x - x')$$

Plane wave basis:
$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} |k\rangle\langle k| = \hat{1}$$

Orthogonality:
$$\langle k' | k \rangle = 2\pi\delta(k - k')$$

Inner product between the basis vectors:
$$\langle x | k \rangle = e^{ikx}$$

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$$|\psi(t)\rangle = \hat{1} |\psi(t)\rangle = \left(\int_{-\infty}^{\infty} dx |x\rangle\langle x| \right) |\psi(t)\rangle = \int_{-\infty}^{\infty} dx |x\rangle\langle x|\psi(t)\rangle = \int_{-\infty}^{\infty} dx \psi(x,t) |x\rangle$$

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Complete Basis Sets in 1D

Lets try to write the components of the vector $|\psi(t)\rangle$ in two different basis:

$$\psi(\mathbf{x}, t) = \langle \mathbf{x} | \psi(t) \rangle \longrightarrow \text{Wavefunction in position basis}$$

$$\psi(\mathbf{k}, t) = \langle \mathbf{k} | \psi(t) \rangle \longrightarrow \text{Wavefunction in plane wave basis}$$

What is the relationship between the wavefunctions in the two basis?

$$\begin{aligned} \psi(\mathbf{k}, t) &= \langle \mathbf{k} | \psi(t) \rangle = \langle \mathbf{k} | \hat{1} | \psi(t) \rangle = \langle \mathbf{k} | \left(\int_{-\infty}^{\infty} d\mathbf{x} | \mathbf{x} \rangle \langle \mathbf{x} | \right) | \psi(t) \rangle \\ &= \int_{-\infty}^{\infty} d\mathbf{x} \langle \mathbf{k} | \mathbf{x} \rangle \psi(\mathbf{x}, t) = \int_{-\infty}^{\infty} d\mathbf{x} e^{-i\mathbf{k}\mathbf{x}} \psi(\mathbf{x}, t) \longrightarrow \text{A Fourier transform !!} \end{aligned}$$

The component of the wavefunction in the plane wave basis is just the Fourier transform of the wavefunction in the position basis !!

Complete Basis Sets in 1D: Momentum Basis

Since momentum is related to the wavevector by just a multiplicative constant:

$$p = \hbar k$$

We define a **momentum basis** as:

$$|p\rangle = \frac{1}{\sqrt{\hbar}} |k = p/\hbar\rangle$$

$$\Rightarrow \langle x | p \rangle = \frac{1}{\sqrt{\hbar}} \langle x | k = p/\hbar \rangle = \frac{e^{i \frac{p}{\hbar} x}}{\sqrt{\hbar}}$$

This $\sqrt{\hbar}$ is just a convention

Then:

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} |k\rangle \langle k| = \hat{1}$$

$$\Rightarrow \int_{-\infty}^{\infty} \frac{d(\hbar k)}{2\pi} \frac{1}{\sqrt{\hbar}} |k\rangle \langle k| \frac{1}{\sqrt{\hbar}} = \int_{-\infty}^{\infty} \frac{dp}{2\pi} |p\rangle \langle p| = \hat{1}$$

Completeness of the momentum basis

$$\langle k' | k \rangle = 2\pi \delta(k - k')$$

$$\Rightarrow \frac{1}{\sqrt{\hbar}} \langle k' | k \rangle \frac{1}{\sqrt{\hbar}} = 2\pi \frac{1}{\hbar} \delta(k - k') = 2\pi \delta(\hbar k - \hbar k')$$

$$\Rightarrow \langle p' | p \rangle = 2\pi \delta(p - p') \longrightarrow \text{Orthogonality}$$

$$\psi(p, t) = \langle p | \psi(t) \rangle$$

Complete Basis Sets in 1D: Momentum Basis

Wavefunction in the momentum basis is:

$$\psi(p, t) = \langle p | \psi(t) \rangle = \langle p | \hat{1} | \psi(t) \rangle = \langle p | \left(\int_{-\infty}^{\infty} dx |x\rangle \langle x| \right) | \psi(t) \rangle$$

$$= \int_{-\infty}^{\infty} dx \langle p | x \rangle \psi(x, t) = \int_{-\infty}^{\infty} dx \frac{e^{-i\frac{p}{\hbar}x}}{\sqrt{\hbar}} \psi(x, t) \longrightarrow \text{Again a Fourier transform}$$

Mean Values or Expectation Values of Observables in 1D

Position:

$$\langle \mathbf{x} \rangle(t) = \int_{-\infty}^{\infty} d\mathbf{x} \psi^*(\mathbf{x}, t) [\mathbf{x}] \psi(\mathbf{x}, t)$$

Potential Energy:

$$\langle \mathbf{PE} \rangle(t) = \langle \mathbf{V}(\mathbf{x}) \rangle(t) = \int_{-\infty}^{\infty} d\mathbf{x} \psi^*(\mathbf{x}, t) [\mathbf{V}(\mathbf{x})] \psi(\mathbf{x}, t)$$

Momentum:

$$\langle \mathbf{p} \rangle(t) = \int_{-\infty}^{\infty} d\mathbf{x} \psi^*(\mathbf{x}, t) \left[\frac{\hbar}{i} \frac{\partial}{\partial \mathbf{x}} \right] \psi(\mathbf{x}, t)$$

Kinetic Energy:

$$\langle \mathbf{KE} \rangle(t) = \int_{-\infty}^{\infty} d\mathbf{x} \psi^*(\mathbf{x}, t) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}^2} \right] \psi(\mathbf{x}, t)$$

Total Energy:

$$\langle \mathbf{E} \rangle(t) = \int_{-\infty}^{\infty} d\mathbf{x} \psi^*(\mathbf{x}, t) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}^2} + \mathbf{V}(\mathbf{x}) \right] \psi(\mathbf{x}, t)$$

These are all
basis dependent
expressions!

The Momentum Operator in 1D

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{\hbar}} \psi(p,t) \quad \Leftrightarrow \quad \psi(p,t) = \int_{-\infty}^{\infty} dx \frac{e^{-i\frac{p}{\hbar}x}}{\sqrt{\hbar}} \psi(x,t)$$

Consider the expectation value:

$$\langle p \rangle(t) = \int_{-\infty}^{\infty} dx \psi^*(x,t) \left[\frac{\hbar}{i} \frac{\partial}{\partial x} \right] \psi(x,t)$$

We will now write it in a different way:

$$\begin{aligned} \langle p \rangle(t) &= \int_{-\infty}^{\infty} dx \psi^*(x,t) \left[\frac{\hbar}{i} \frac{\partial}{\partial x} \right] \psi(x,t) \\ &= \int_{-\infty}^{\infty} dx \left[\int_{-\infty}^{\infty} \frac{dp'}{2\pi} \frac{e^{-i\frac{p'}{\hbar}x}}{\sqrt{\hbar}} \right] \left[\frac{\hbar}{i} \frac{\partial}{\partial x} \right] \left[\int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{\hbar}} \psi(p,t) \right] \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \int_{-\infty}^{\infty} \frac{dp'}{2\pi} \int_{-\infty}^{\infty} dx \psi^*(p',t) \frac{e^{-i\frac{p'}{\hbar}x}}{\sqrt{\hbar}} \left[\frac{\hbar}{i} \frac{\partial}{\partial x} \right] \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{\hbar}} \psi(p,t) \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \int_{-\infty}^{\infty} \frac{dp'}{2\pi} \int_{-\infty}^{\infty} dx \psi^*(p',t) p \frac{e^{i\frac{(p-p')}{\hbar}x}}{\hbar} \psi(p,t) \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \int_{-\infty}^{\infty} \frac{dp'}{2\pi} \psi^*(p',t) p \frac{2\pi\hbar\delta(p-p')}{\hbar} \psi(p,t) \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \psi^*(p,t) p \psi(p,t) \end{aligned}$$

The Momentum Operator in 1D

$$\langle p \rangle(t) = \int_{-\infty}^{\infty} dx \psi^*(x,t) \left[\frac{\hbar}{i} \frac{\partial}{\partial x} \right] \psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \psi^*(p,t) p \psi(p,t)$$

The quantity we are trying to find is the same, but the appearance of the expression changes depending on the basis used (position basis or the momentum basis)

Can we write this in a basis-independent way???. The answer is yes!!

$$\langle p \rangle(t) = \langle \psi(t) | \hat{p} | \psi(t) \rangle$$



But what is this operator?

The Momentum Operator in 1D

Momentum operator \hat{p} has the following properties:

1) $\hat{p}|p'\rangle = p'|p'\rangle \longrightarrow$ momentum basis are eigenstates of the momentum operator

2) $\hat{p} = \hat{p}^\dagger \longrightarrow$ Momentum operator is Hermitian (or self-adjoint)

$$3) \langle x | \hat{p} | \psi(t) \rangle = \langle x | \hat{p} \hat{1} | \psi(t) \rangle = \langle x | \hat{p} \left(\int_{-\infty}^{\infty} \frac{dp}{2\pi} |p\rangle \langle p| \right) | \psi(t) \rangle$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \langle x | \hat{p} | p \rangle \psi(p, t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} p \langle x | p \rangle \psi(p, t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} p \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{\hbar}} \psi(p, t)$$

$$= \frac{\hbar}{i} \frac{\partial}{\partial x} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{\hbar}} \psi(p, t) = \frac{\hbar}{i} \frac{\partial \psi(x, t)}{\partial x} \longrightarrow$$

The action of momentum operator is a derivative in the position representation

The Momentum Operator in 1D

$$4) \langle p | \hat{p} | \psi(t) \rangle = \left(\langle \psi(t) | \hat{p}^\dagger | p \rangle \right)^* = \left(\langle \psi(t) | \hat{p} | p \rangle \right)^* = \left(p \langle \psi(t) | p \rangle \right)^* = p \langle p | \psi(t) \rangle = p \psi(p, t)$$

→ The action of momentum operator in momentum basis is just a multiplication

$$5) \hat{p} = \hat{1} \hat{p} \hat{1} = \left(\int_{-\infty}^{\infty} \frac{dp}{2\pi} |p\rangle \langle p| \right) \hat{p} \left(\int_{-\infty}^{\infty} \frac{dp'}{2\pi} |p'\rangle \langle p'| \right) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \int_{-\infty}^{\infty} \frac{dp'}{2\pi} \langle p | \hat{p} | p' \rangle |p'\rangle \langle p|$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \int_{-\infty}^{\infty} \frac{dp'}{2\pi} p' \langle p | p' \rangle |p'\rangle \langle p| = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \int_{-\infty}^{\infty} \frac{dp'}{2\pi} p' (2\pi) \delta(p - p') |p'\rangle \langle p|$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} p |p\rangle \langle p| \quad \longrightarrow \quad \text{Any operator is diagonal in the basis formed by its own eigenvectors}$$

Finally, the expectation value of the momentum becomes:

$$\langle p \rangle(t) = \int_{-\infty}^{\infty} dx \psi^*(x, t) \left[\frac{\hbar}{i} \frac{\partial}{\partial x} \right] \psi(x, t) = \int_{-\infty}^{\infty} dx \psi^*(x, t) \langle x | \hat{p} | \psi(t) \rangle$$

$$= \int_{-\infty}^{\infty} dx \langle \psi(t) | x \rangle \langle x | \hat{p} | \psi(t) \rangle = \langle \psi(t) | \left(\int_{-\infty}^{\infty} dx |x\rangle \langle x| \right) \hat{p} | \psi(t) \rangle$$

$$= \langle \psi(t) | \hat{1} \hat{p} | \psi(t) \rangle$$

$$= \langle \psi(t) | \hat{p} | \psi(t) \rangle$$

The Momentum Operator in 1D

6) Lets check out the eigenstates of the momentum operator:

$$\hat{p}|\mathbf{p}'\rangle = \mathbf{p}'|\mathbf{p}'\rangle$$

Suppose the **quantum state** of a particle is the eigenstate of the momentum operator:

$$|\psi\rangle = |\mathbf{p}'\rangle$$

Then what is the **wavefunction** of the particle?

$$\psi(\mathbf{x}) = \langle \mathbf{x} | \psi \rangle = \langle \mathbf{x} | \mathbf{p}' \rangle = \frac{e^{i\frac{\mathbf{p}'}{\hbar}\mathbf{x}}}{\sqrt{\hbar}} \longrightarrow \text{A plane wave with wavevector } \mathbf{p}'/\hbar$$

Thus, plane waves are wavefunctions of the eigenstates of the momentum operator!

The Momentum Operator in 1D

7) Lets check out the eigenstates of the momentum operator once more:

$$\hat{p}|\mathbf{p}'\rangle = \mathbf{p}'|\mathbf{p}'\rangle$$

We see this (or project this) equation in the position basis:

$$\begin{aligned}\langle \mathbf{x} | \hat{p} | \mathbf{p}' \rangle &= \mathbf{p}' \langle \mathbf{x} | \mathbf{p}' \rangle \\ \Rightarrow \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{x}} \langle \mathbf{x} | \mathbf{p}' \rangle &= \mathbf{p}' \langle \mathbf{x} | \mathbf{p}' \rangle\end{aligned}$$

If you didn't know what $\langle \mathbf{x} | \mathbf{p}' \rangle$ was, you can conclude from the above eigenvalue equation that:

$$\langle \mathbf{x} | \mathbf{p}' \rangle \propto e^{i \frac{\mathbf{p}'}{\hbar} \mathbf{x}}$$

The Position Operator in 1D

We need to write the following in a basis-independent way:

$$\langle \mathbf{x} \rangle(t) = \int_{-\infty}^{\infty} d\mathbf{x} \psi^*(\mathbf{x}, t) [\mathbf{x}] \psi(\mathbf{x}, t)$$

Answer:

$$\langle \mathbf{x} \rangle(t) = \langle \psi(t) | \hat{\mathbf{x}} | \psi(t) \rangle$$

Here $\hat{\mathbf{x}}$ is the position operator with the following properties:

- 1) $\hat{\mathbf{x}} | \mathbf{x}' \rangle = \mathbf{x}' | \mathbf{x}' \rangle$ \longrightarrow position basis are eigenstates of the position operator
- 2) $\hat{\mathbf{x}} = \hat{\mathbf{x}}^\dagger$ \longrightarrow Position operator is Hermitian (or self-adjoint)
- 3) $\hat{\mathbf{x}} = \int_{-\infty}^{\infty} d\mathbf{x} \mathbf{x} | \mathbf{x} \rangle \langle \mathbf{x} |$ \longrightarrow Any operator is diagonal in the basis formed by its own eigenvectors

$$\begin{aligned} 4) \langle \mathbf{x} \rangle(t) &= \langle \psi(t) | \hat{\mathbf{x}} | \psi(t) \rangle = \langle \hat{\mathbf{x}} \rangle(t) = \langle \psi(t) | \left(\int_{-\infty}^{\infty} d\mathbf{x} \mathbf{x} | \mathbf{x} \rangle \langle \mathbf{x} | \right) | \psi(t) \rangle \\ &= \int_{-\infty}^{\infty} d\mathbf{x} \langle \psi(t) | \mathbf{x} \rangle \mathbf{x} \langle \mathbf{x} | \psi(t) \rangle = \int_{-\infty}^{\infty} d\mathbf{x} \psi^*(\mathbf{x}, t) \mathbf{x} \psi(\mathbf{x}, t) \end{aligned}$$

The Energy Operator, or the Hamiltonian, in 1D

We need to write the following in a basis-independent way:

$$\langle E \rangle(t) = \int_{-\infty}^{\infty} dx \psi^*(x, t) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t)$$

Answer:

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

Here \hat{H} is the Hamiltonian operator which can be written in terms of the momentum and position operators:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

1) $\hat{H} = \hat{H}^\dagger$ \longrightarrow **Hamiltonian operator is Hermitian (or self-adjoint)**

$$\begin{aligned} 2) \langle \hat{H} \rangle(t) &= \langle \psi(t) | \hat{H} | \psi(t) \rangle = \langle \psi(t) | \frac{\hat{p}^2}{2m} + V(\hat{x}) | \psi(t) \rangle = \langle \psi(t) | \hat{1} \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) \right) | \psi(t) \rangle \\ &= \langle \psi(t) | \left(\int_{-\infty}^{\infty} dx |x\rangle \langle x| \right) \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) \right) | \psi(t) \rangle = \int_{-\infty}^{\infty} dx \langle \psi(t) | x \rangle \langle x | \frac{\hat{p}^2}{2m} + V(\hat{x}) | \psi(t) \rangle \\ &= \int_{-\infty}^{\infty} dx \psi^*(x, t) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t) \end{aligned}$$

The Eigenstates and Eigenvalues of the Hamiltonian

3) Wouldn't it be nice to also know ALL the eigenstates of the Hamiltonian operator:

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

Lets see this equation (or project this equation) in the position basis:

$$\langle \mathbf{x} | \hat{H} | \phi \rangle = E \langle \mathbf{x} | \phi \rangle$$

$$\Rightarrow \langle \mathbf{x} | \frac{\hat{p}^2}{2m} + V(\hat{\mathbf{x}}) | \phi \rangle = E \langle \mathbf{x} | \phi \rangle$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}^2} + V(\mathbf{x}) \right] \phi(\mathbf{x}) = E \phi(\mathbf{x}) \longrightarrow \text{The time-independent Schrödinger equation!!}$$

Solutions of the time-independent Schrödinger equation are the eigenfunctions of the Hamiltonian in the position basis

Suppose the eigenvectors and eigenvalues are:

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}^2} + V(\mathbf{x}) \right] \phi_j(\mathbf{x}) = E_j \phi_j(\mathbf{x})$$

In basis-independent notation:

$$\hat{H}|\phi_j\rangle = E_j|\phi_j\rangle$$

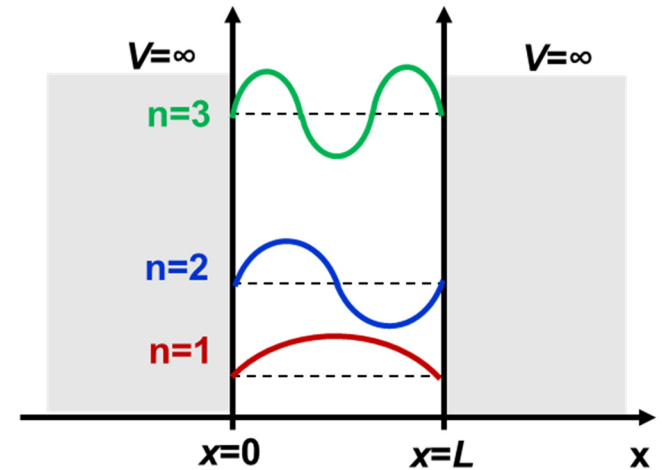
The Eigenstates and Eigenvalues of the Hamiltonian

Recall how we had solved the Hamiltonian eigenvalue equation for an infinite potential well:

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$$

$$\Rightarrow \langle \mathbf{x} | \hat{H} | \phi_n \rangle = E_n \langle \mathbf{x} | \phi_n \rangle$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}^2} + V(\mathbf{x}) \right] \phi_n(\mathbf{x}) = E_n \phi_n(\mathbf{x})$$



Solutions of the time-independent Schrödinger equation are the eigenfunctions of the Hamiltonian in the position basis

Schrödinger Equation Revisited: The Basis-Independent Form

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\mathbf{x}, t)}{\partial \mathbf{x}^2} + V(\mathbf{x})\psi(\mathbf{x}, t)$$

We can write the above equation as:

$$i\hbar \frac{\partial}{\partial t} \langle \mathbf{x} | \psi(t) \rangle = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}^2} + V(\mathbf{x}) \right] \langle \mathbf{x} | \psi(t) \rangle$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \langle \mathbf{x} | \psi(t) \rangle = \langle \mathbf{x} | \frac{\hat{p}^2}{2m} + V(\hat{\mathbf{x}}) | \psi(t) \rangle$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \langle \mathbf{x} | \psi(t) \rangle = \langle \mathbf{x} | \hat{H} | \psi(t) \rangle$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} | \psi(t) \rangle = \hat{H} | \psi(t) \rangle$$

This is the more general basis-independent form of the Schrödinger equation!

$$i\hbar \frac{\partial}{\partial t} | \psi(t) \rangle = \hat{H} | \psi(t) \rangle$$

The Eigenstates and Eigenvalues of the Hamiltonian

4) The eigenstates of a Hermitian operator always form a complete set, and therefore:

$$\sum_j |\phi_j\rangle\langle\phi_j| = \hat{1}$$

5)
$$\hat{H} = \hat{1} \hat{H} \hat{1} = \left(\sum_j |\phi_j\rangle\langle\phi_j| \right) \hat{H} \left(\sum_m |\phi_m\rangle\langle\phi_m| \right) = \sum_{j,m} \langle\phi_j| \hat{H} |\phi_m\rangle |\phi_j\rangle\langle\phi_m|$$

$$= \sum_{j,m} E_m \langle\phi_j|\phi_m\rangle |\phi_j\rangle\langle\phi_m| = \sum_{j,m} E_m \delta_{jm} |\phi_j\rangle\langle\phi_m|$$

$$= \sum_j E_j |\phi_j\rangle\langle\phi_j| \longrightarrow \text{Of course, any Hermitian operator is diagonal in the basis formed by its own eigenvectors}$$

If we make the following mapping from the Hilbert space of the Hamiltonian eigenstates to the Hilbert space of column vectors:

$$|\phi_1\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} \quad |\phi_2\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} \quad |\phi_3\rangle \rightarrow \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} \quad \dots$$

Then in this chosen column vector Hilbert space, the Hamiltonian operator is the following *infinite* matrix:

$$\hat{H} \rightarrow \begin{bmatrix} E_1 & 0 & 0 & 0 & \dots & \dots \\ 0 & E_2 & 0 & 0 & \dots & \dots \\ 0 & 0 & E_3 & 0 & \dots & \dots \\ 0 & 0 & 0 & \ddots & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Operators in 1D

Position:

$$\hat{x} \longrightarrow \begin{aligned} \hat{x} |x'\rangle &= x' |x'\rangle \\ \langle x' | x \rangle &= \delta(x' - x) \end{aligned} \quad \int_{-\infty}^{\infty} dx |x\rangle \langle x| = \hat{1}$$

Potential Energy:

$$V(\hat{x})$$

Momentum:

$$\hat{p} \longrightarrow \begin{aligned} \hat{p} |p'\rangle &= p' |p'\rangle \\ \langle p' | p \rangle &= 2\pi\delta(p - p') \end{aligned} \quad \int_{-\infty}^{\infty} \frac{dp}{2\pi} |p\rangle \langle p| = \hat{1}$$

Kinetic Energy:

$$\frac{\hat{p}^2}{2m}$$

Total Energy:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \longrightarrow \begin{aligned} \hat{H} |\phi_j\rangle &= E_j |\phi_j\rangle \\ \langle \phi_k | \phi_j \rangle &= \delta_{jk} \end{aligned} \quad \sum_j |\phi_j\rangle \langle \phi_j| = \hat{1}$$

When Momentum Eigenstates are also Energy Eigenstates

Total Energy:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad \longrightarrow \quad \begin{aligned} \hat{H}|\phi_j\rangle &= E_j|\phi_j\rangle \\ \langle\phi_k|\phi_j\rangle &= \delta_{jk} \end{aligned} \quad \sum_j |\phi_j\rangle\langle\phi_j| = \hat{1}$$

What if the potential energy is zero (or constant U) ??

$$\hat{H} = \frac{\hat{p}^2}{2m} + U$$

Then momentum eigenstates are also energy eigenstates:

$$\hat{H}|p\rangle = \left(\frac{\hat{p}^2}{2m} + U \right) |p\rangle = \left(\frac{p^2}{2m} + U \right) |p\rangle$$

and Hamiltonian and the momentum operator have a common set of eigenstates!!

Note that in this case:

$$[\hat{H}, \hat{p}] = 0$$

Operators in 3D

Position (vector operator):

$$\hat{\vec{r}} = \hat{x}\mathbf{e}_x + \hat{y}\mathbf{e}_y + \hat{z}\mathbf{e}_z \quad \longrightarrow$$

$$\hat{\vec{r}}|\vec{r}'\rangle = \vec{r}'|\vec{r}'\rangle$$

$$\langle\vec{r}'|\vec{r}\rangle = \delta^3(\vec{r}' - \vec{r})$$

$$\int d^3\vec{r} |\vec{r}\rangle\langle\vec{r}| = \hat{1}$$

Potential Energy (scalar operator):

$$V(\hat{\vec{r}})$$

Momentum (vector operator):

$$\hat{\vec{p}} = \hat{p}_x\mathbf{e}_x + \hat{p}_y\mathbf{e}_y + \hat{p}_z\mathbf{e}_z \quad \longrightarrow$$

$$\hat{\vec{p}}|\vec{p}'\rangle = \vec{p}'|\vec{p}'\rangle$$

$$\langle\vec{p}'|\vec{p}\rangle = (2\pi)^3 \delta^3(\vec{p}' - \vec{p})$$

$$\int \frac{d^3\vec{p}}{(2\pi)^3} |\vec{p}\rangle\langle\vec{p}| = \hat{1}$$

Kinetic Energy (scalar operator):

$$\frac{\hat{\vec{p}} \cdot \hat{\vec{p}}}{2m} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m}$$

Total Energy (scalar operator):

$$\hat{H} = \frac{\hat{\vec{p}} \cdot \hat{\vec{p}}}{2m} + V(\hat{\vec{r}}) \quad \longrightarrow$$

$$\hat{H}|\phi_j\rangle = E_j|\phi_j\rangle$$

$$\langle\phi_k|\phi_j\rangle = \delta_{jk}$$

$$\sum_j |\phi_j\rangle\langle\phi_j| = \hat{1}$$

