LECTURE 22: The QM Postulates

What I expect you to learn:

- What are the QM postulates
- How to work with the Dirac notation

(Corresponds to sections 5.1-5.4 of textbook)

(Problem set 3 due Friday!)

THE POSTULATES OF QM

In classical physics, the state of a system can be determined at each instant by dynamical variables (position, momentum vectors, etc). In principle, they can be measured simultaneously to arbitrary precision.

In QM, the situation is completely different: in general when a dynamical variable is measured, the system is modified in an unpredictable way. What QM can predict is the probablility of a measurement's outcome.

Also in QM, Heisenberg's uncertainty relations set a limit on the precision with which one can measure two given variables at the same time.

QM is based on a set of postulates that have not been derived*. They are justified by experimental results.

$\boxed{\text{THE POSTULATES OF QM}}$

Postulate 1: The state of a physical system is specified by a state vector (in a Hilbert space) at each time t: $|\psi(t)\rangle$

-The Hilbert space is linear and there is a scalar product in the vector space which can be expressed as:

$$\int_{-\infty}^{\infty} \varphi^*(x)\,\psi(x)\,dx$$

The vector space in generally complex, infinite-dimensional, continuous (since x is continuous).

Linear $\rightarrow$ Superposition principle

$|\psi_1\rangle$ is a vector, $|\psi_2\rangle$ is a vector in that space then

$|\psi_3\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$ is also a vector

↳ complex constant

THE POSTULATES OF QM

SCALAR PRODUCT (OR INNER PRODUCT) FOR VECTORS IN 3D:

$$\vec{r} \cdot \vec{s} = r_1 \cdot s_1 + r_2 \cdot s_2 + r_3 \cdot s_3 = \text{real number}$$

$$\vec{r} = (r_1, r_2, r_3) \quad , \quad \vec{s} = (s_1, s_2, s_3)$$

we could write $\vec{r} \cdot \vec{s}$ as (r, s)

For a orthogonal basis of vectors in 3D

e.g $\hat{x}, \hat{y}, \hat{z}$, we have

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

A 3D vector $\vec{r}$ can be written as

$$\vec{r} = \alpha \hat{x} + \beta \hat{y} + \gamma \hat{z}$$

, if $\hat{x}, \hat{y}, \hat{z}$ are orthogonal and form a complete basis

THE POSTULATES OF QM

FOR THE VECTOR SPACE OF QM, WE DEFINE AN INNER PRODUCT THAT WE WILL WRITE $\langle \varphi | \psi \rangle$ (We could have used $\varphi \cdot \psi$ or (φ, ψ))

$\langle \varphi | \psi \rangle = c$, a complex number

We also have the following relations:

$$\langle \psi + \varphi | \theta \rangle = \langle \psi | \theta \rangle + \langle \varphi | \theta \rangle$$
$$\langle \psi | c\varphi \rangle = c \langle \psi | \varphi \rangle$$
$$\langle \psi | \varphi \rangle = \langle \varphi | \psi \rangle^*$$
$$\langle \psi | \psi \rangle \geq 0$$

$\rightarrow$ wave function normalization implies $\langle \psi | \psi \rangle = 1$

ψ_1 an ψ_2 are orthogonal if $\langle \psi_1, \psi_2 \rangle = 0$

THE POSTULATES OF QM

Postulate 2: to every physically measurable quantity A (that we will call observable) there corresponds a linear Hermitian operator A whose eigenvectors form a complete basis.

Postulate 3: The measurement of an observable A yields one of the eigenvalues of the linear operator A associated with A.

- Linear operator: $A(c_1|\psi_1\rangle + c_2|\psi_2\rangle)$
$$= c_1 A|\psi_1\rangle + c_2 A|\psi_2\rangle$$

- Hermitian: $\langle\varphi|(A\psi)\rangle = \langle(A\varphi)|\psi\rangle$
$$\langle\varphi|(A\psi)\rangle \equiv \langle\varphi|A|\psi\rangle$$

i.e $A^{T} = A$

Hermitian operators have real eigenvalues

THE POSTULATES OF QM

In wave mechanics we had for Hermitian conjugates:

$$\int_{-\infty}^{\infty} dx\, (\hat{A}\varphi(x))^* \psi(x) = \int_{-\infty}^{\infty} dx\, \varphi(x)^* \hat{A}^+ \psi(x)$$

i.e.

$$\langle \hat{A}\varphi | \psi \rangle = \langle \varphi | \hat{A}^+ | \psi \rangle \Rightarrow \langle \varphi | \hat{A}^+ | \psi \rangle^* = \langle \hat{A}\varphi | \psi \rangle^*$$

remember that $\langle \varphi | \psi \rangle^* = \langle \psi | \varphi \rangle$, so $\quad = \langle \psi | \hat{A} | \varphi \rangle$

Exercise: Show that the eigenvectors of a Hermitian operator are orthogonal if their eigenvalues are different

i.e.

$$\hat{O}|a\rangle = a|a\rangle$$
$$\hat{O}|b\rangle = b|b\rangle$$

$$\Rightarrow \langle b | a \rangle = 0$$

THE POSTULATES OF QM

– A complete basis: $A|\psi_n\rangle = a_n|\psi_n\rangle$

We can write $|\psi\rangle = \sum_n a_n|\psi_n\rangle$

i.e $|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle + \ldots$

$$\langle\psi_1|\psi\rangle = \langle\psi_1|a_1\psi_1\rangle + \langle\psi_1|a_2\psi_2\rangle + \ldots = a_1$$

$$a_n = \langle\psi_n|\psi\rangle$$

Example in 3D: $\vec{x} = (1,0,0)$, $\vec{r}(3,4,5)$

$$\vec{x}\cdot\vec{r} = (\vec{x},\vec{r}) = 3$$

if ψ_n is an eigenvector of $\hat{A}$ with eigenvalue a_n,
Then:

$$\langle\psi_n|\hat{A}|\psi_n\rangle = \langle\psi_n|a_n|\psi_n\rangle = a_n\langle\psi_n|\psi_n\rangle = a_n$$

* the eigenvector basis for an operator can be discrete or continuous ($\hat{x}$ operator)

THE POSTULATES OF QM

Postulate 4: (part 1) if a series measurements of the observable A is performed on an ensemble of systems described by $|\psi\rangle$, the average value will be given by:

$$\langle A\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}$$

NOTES: UNITARY OPERATORS

A linear operator $\hat{U}$ is unitary if $\hat{U}\hat{U}^{\dagger} = I$

We can express $\hat{U}$ as $\hat{U} = e^{i\hat{A}}$

PROJECTION OPERATORS

If $\hat{\Lambda}$ is a Hermitian operator with the following property: $\hat{\Lambda}^2 = \Lambda$, then $\hat{\Lambda}$ is a projection operator.

THE POSTULATES OF QM

PROJECTION OPs (cont.)

$|\psi_n\rangle\langle\psi_n|$ is a projection operator

$$|\psi_n\rangle\langle\psi_n|\psi\rangle = a_n|\psi_n\rangle$$

$$\sum_n |\psi_n\rangle\langle\psi_n| = \hat{I}$$

$\hookrightarrow$ completeness relation

We can write $|\psi\rangle$ as:

$$\boxed{|\psi\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle}$$

THE POSTULATES OF QM

Postulate 4 (part 2): WHEN MEASURING OBSERVABLE A OF A SYSTEM IN STATE VECTOR $|\psi\rangle$, THE PROBABILITY OF OF MEASURING AN EIGENVALUE IS GIVEN BY:

→ discrete, non-degenerate eigenvalues

$$P_n(a_n) = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|a_n|^2}{\langle\psi|\psi\rangle}$$

→ discrete, m-degenerate

$$P_n(a_n) = \sum_{i=1}^{m} \frac{|\langle\psi_n^i|\psi\rangle|^2}{\langle\psi|\psi\rangle}$$

→ continuous:

$$\frac{dP(a)}{da} = \frac{|\psi(a)|^2}{\langle\psi|\psi\rangle} = \frac{|\psi(a)|^2}{\int_{-\infty}^{\infty} |\psi(a')|\, da'}$$

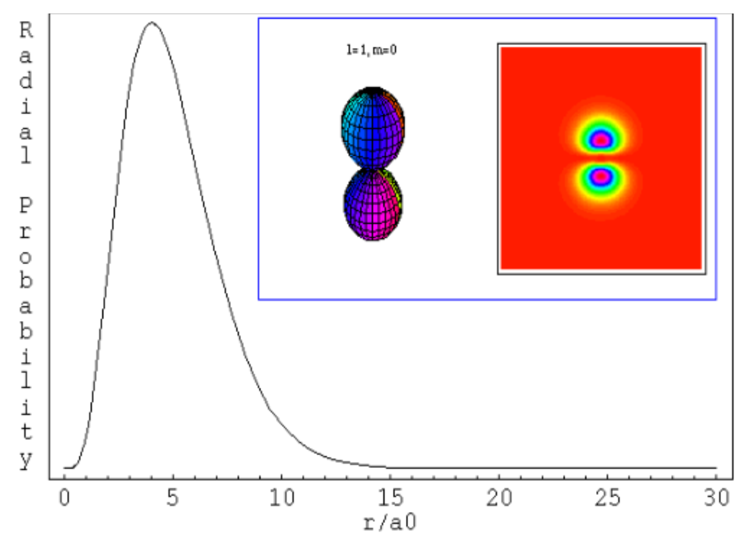
THE POSTULATES OF QM

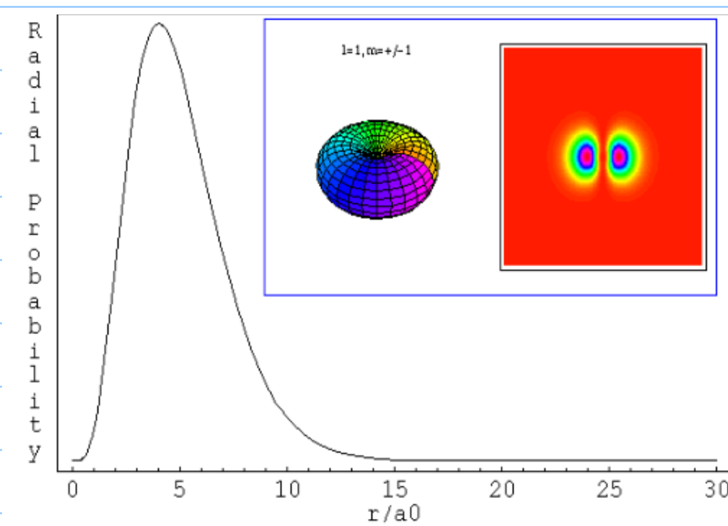
Degeneracy: if a number of different eigenvectors have the same eigenvalue, then this eigenvalue is said to be degenerate

Example: 2^{nd} energy level of the hydrogen atom:

$\psi_2(r, \theta, \varphi)$:

some p orbitals:





THE POSTULATES OF QM

Continuous eigenvalues:

$$\hat{x}|x\rangle = x|x\rangle$$

We can expand $|\psi\rangle$ with those eigenvectors

$$|\psi\rangle = \int_{-\infty}^{\infty} dx \; c(x)\,|x\rangle \qquad (1)$$

using orthonormality of $|x\rangle$ eigenstates:

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

let's multiply (1) by $\langle x'|$:

$$\langle x'|\psi\rangle = \int_{-\infty}^{\infty} dx \; \langle x'|x\rangle \, c(x) = \int_{-\infty}^{\infty} \delta(x-x')\, c(x)\, dx$$

$$= c(x') \quad , \quad |c(x')|^2 = |\psi(x')|^2$$

$$\boxed{\langle x'|\psi\rangle = \psi(x')}$$

THE POSTULATES OF QM

So we have $\psi(x) = \langle x | \psi \rangle$

$\Rightarrow \quad \varphi(p) = \langle p | \psi \rangle$

→ completeness relation for position eigenkets:

$$\int_{-\infty}^{\infty} dx \, |x\rangle\langle x| = 1 \qquad (2)$$

we can insert (2) in $\langle \psi | \varphi \rangle$:

$$\langle \psi | \varphi \rangle = \langle \psi | 1 | \varphi \rangle = \int_{-\infty}^{\infty} \langle \psi | x \rangle \langle x | \varphi \rangle \, dx$$

$$= \int_{-\infty}^{\infty} \psi(x)^* \varphi(x) \, dx$$

or: $\langle A\varphi | \psi \rangle = \int_{-\infty}^{\infty} dx \, (A\varphi(x))^* \psi(x)$

THE POSTULATES OF QM

Recall: $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\, \varphi(p)\, e^{ipx/\hbar}$

$$\psi(x) = \langle x | \psi \rangle = \int_{-\infty}^{\infty} dp\, \langle x | p \rangle \langle p | \psi \rangle = \int_{-\infty}^{\infty} dp\, \langle x | p \rangle\, \varphi(p)$$

$$\Rightarrow \langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}$$

Don't confuse $\hat{x}$ with $|x\rangle$, or $\langle x \rangle$!

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

$\hat{x} | x \rangle = x | x \rangle$

THE POSTULATES OF QM

We'll look at the link between commutators and the uncertainty relations:

In statistics the variance is expressed as

$$\text{var} = \frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2$$

the standard deviation $\sigma = \sqrt{\text{var}}$

We'll use σ as our definition of width:

$$\Delta A = \sqrt{\langle (A - \langle A\rangle)^2\rangle} \quad , \quad \Delta B = \sqrt{\langle (B - \langle B\rangle)^2\rangle}$$

$$(\Delta A)^2 = \langle (A - \langle A\rangle)^2\rangle = \langle A^2\rangle - \langle A\rangle^2 \quad *$$

We want to show that $\Delta A \Delta B \geq \frac{1}{2}|\langle [A,B]\rangle|$

THE POSTULATES OF QM

We'll set: $\bar{A} = A - \langle A \rangle$, $\bar{A}$ lin. hermitian

$\bar{B} = B - \langle B \rangle$, $\bar{B}$ " "

$$\Rightarrow (\Delta A)^2 = \langle \bar{A}^2 \rangle \ , \ (\Delta B)^2 = \langle \bar{B}^2 \rangle$$

$$[\bar{A}, \bar{B}] = [A - \langle A \rangle, B - \langle B \rangle] = [A, B]$$

Let's introduce the linear operator $C = \bar{A} + i\lambda \bar{B}$ where λ is a real constant

$$\langle C C^{\dagger} \rangle \geq 0 \quad = \langle \psi | C C^{\dagger} | \psi \rangle = \langle C^{\dagger}\psi | C^{\dagger}\psi \rangle \geq 0$$

$$\langle (\bar{A} + i\lambda \bar{B}) (\bar{A} - i\lambda \bar{B}) \rangle = \langle \bar{A}^2 + \lambda^2 \bar{B}^2 - i\lambda [A, B] \rangle$$

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 - i\lambda \langle [A, B] \rangle = F(\lambda)$$

minimum of $F(\lambda)$ for $\frac{dF(\lambda)}{d\lambda} = 0$

$$\Rightarrow 2\lambda (\Delta B)^2 - i \langle [A, B] \rangle = 0 \ , \quad \lambda_{min} = \frac{i}{2} \frac{\langle [A, B] \rangle}{(\Delta B)^2}$$

THE POSTULATES OF QM

$$F(\lambda_{min}) = (\Delta A)^2 + -\frac{1}{4}\frac{\langle [A,B]\rangle^2}{(\Delta B)^4}\cdot(\Delta B)^2 + \frac{1}{2}\frac{\langle [A,B]\rangle}{(\Delta B)^2}\langle [A,B]\rangle$$

$$= (\Delta A)^2 + \frac{1}{4}\frac{\langle [A,B]\rangle^2}{(\Delta B)^2} \geq 0$$

$$\Rightarrow (\Delta A)^2(\Delta B)^2 \geq -\frac{1}{4}\langle [A,B]\rangle^2$$

For $[A,B] = i\hbar$, we have

$$(\Delta A)^2(\Delta B)^2 \geq -\frac{1}{4}\cdot -\hbar^2$$

$$\boxed{\Rightarrow \Delta A \Delta B \geq \hbar/2}$$

THE POSTULATES OF QM

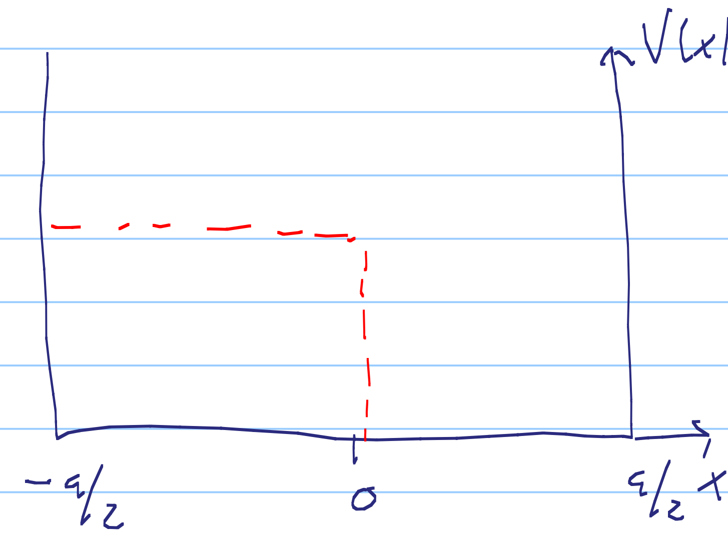
Example Problem: (Q4, midterm 2004)

Particle in infinite well:

Particle is localised in left hand side of the well:

$\psi(x) = \sqrt{\frac{2}{a}}$, $-a/2 < x < 0$

$\psi(x) = 0$, $x \geq 0$



a) will the particle remain localized on left-hand side? why?

b) what is the prob. that an energy measurement will yield the ground state $(n=1)$?

Problem cont.

we have $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ For a well with walls at 0, a. we'll move the wall here...

$P_n = |a_n|^2$, $a_n = \langle \psi_n | \psi \rangle$

$$a_n = \int_{-\infty}^{\infty} \langle \psi_n | x \rangle \langle x | \psi \rangle \, dx = \int_{-\infty}^{\infty} \psi_n(x)^* \psi(x) \, dx$$

$$a_1 = \int_{-\infty}^{\infty} \psi_1(x)^* \psi(x) \, dx = \int_0^{a/2} \frac{2}{a} \sin\frac{\pi x}{a} \, dx$$

$$= -\frac{a}{\pi} \cdot \frac{2}{a} \cdot \cos\frac{\pi x}{a} \Big|_0^{a/2} = 0 - -\frac{2}{\pi}$$

$$|a_1|^2 = \frac{4}{\pi^2} = 0.405 \rightarrow 40.5\%$$