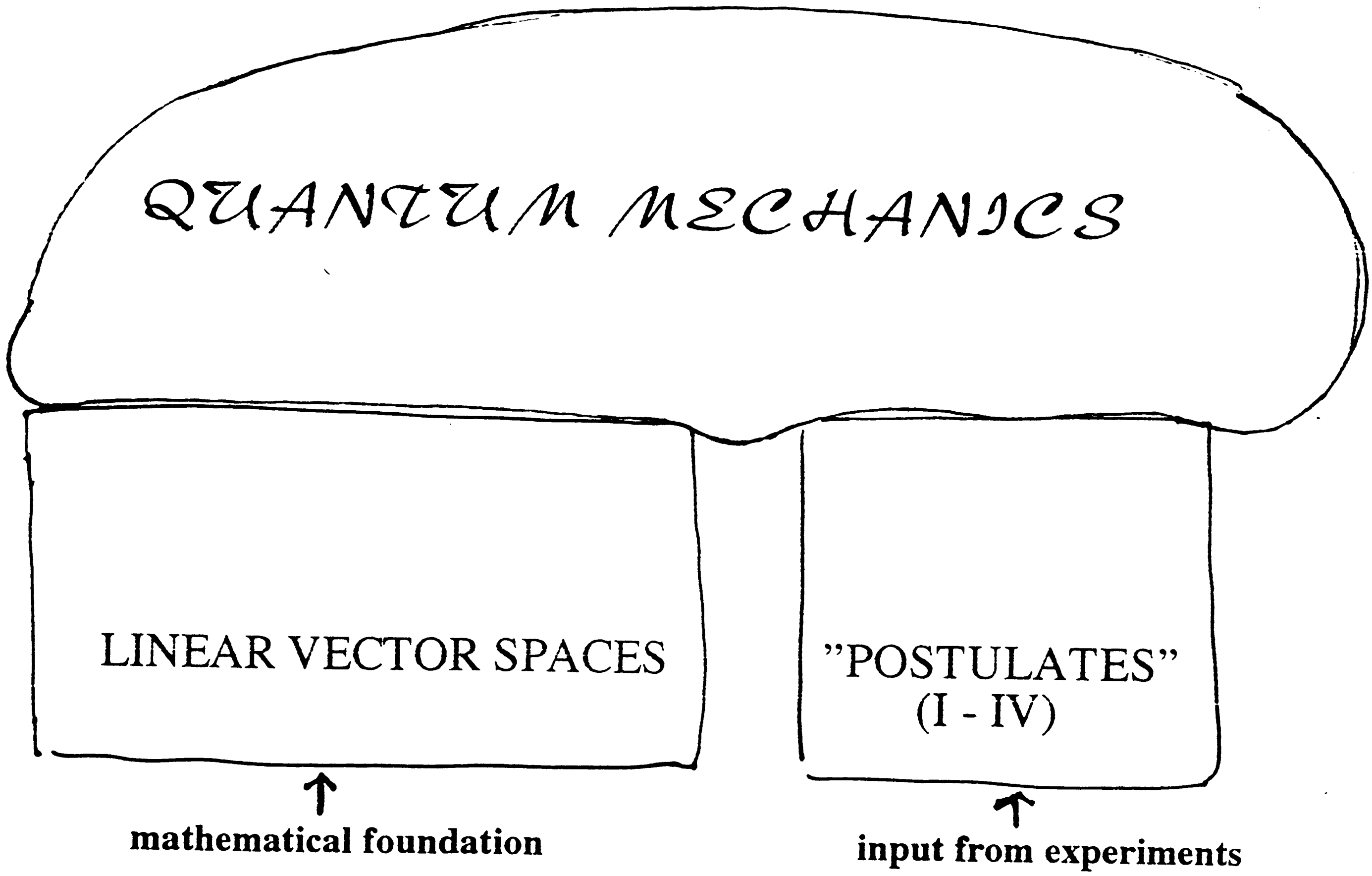
Quantum Mechanics

Second lecture

Sept. 3 2003


QUANTUM MECHANICS
LINEAR VECTOR SPACES
"POSTULATES"
(I - IV)
mathematical foundation
input from experiments

Matrix representation

$$|V\rangle \longrightarrow \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \qquad \text{BASIS} \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \ldots \quad |n\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

$$\langle V| \longrightarrow \begin{pmatrix} v_1^* & v_2^* & \ldots & v_n^* \end{pmatrix}$$

BRA = ADJOINT (= TRANSPOSE CONJUGATE) OF A KET

$|V\rangle$ AND $\langle V|$ BELONG TO DUAL SPACES

$$|V\rangle \overset{DC}{\longleftrightarrow} \langle V|$$

$$a|V\rangle = |aV\rangle \overset{DC}{\longleftrightarrow} (|aV\rangle)^{+} = \langle V|a^* = \langle aV|$$

Expansion in an ON basis

$$|V\rangle = \sum_i v_i |i\rangle$$

$$\langle j|V\rangle = \sum_i v_i \underbrace{\langle j|i\rangle}_{\delta_{ij}} = v_j$$

What is all this good for...?

3 (of the 4) postulates of **quantum mechanics** (roughly) say that

1. PHYSICAL STATES $\longrightarrow$ VECTORS IN A LINEAR (infinite-dimensional) VECTOR SPACE (=Hilbert space)

2. PHYSICAL OBSERVABLES $\longrightarrow$ OPERATORS IN THIS SPACE

3. OUTCOME OF A MEASUREMENT $\rightarrow$ EIGENVALUES TO THE CORRESPONDING OPERATOR

Linear operator Ω

a rule for transforming a given vector $|V\rangle$ into another $|V'\rangle$

$$\Omega|V\rangle = |V'\rangle$$

$$\langle V'|\Omega = \langle V''|$$

- satisfying the "*linearity rules*"

$\Rightarrow$ IF THE ACTION ON THE BASIS VECTORS ARE KNOWN, THE ACTION ON <u>ANY</u> VECTOR IN THE SPACE IS DETERMINED

- *The order of operators is important!*

$$\Lambda\Omega|V\rangle = \Lambda(\Omega|V\rangle) = \Lambda|\Omega V\rangle$$

$$\Omega\Lambda - \Lambda\Omega = [\Omega, \Lambda]$$

COMMUTATOR

Useful identities

$$[\Omega, \Lambda\Theta] = \Lambda[\Omega, \Theta] + [\Omega, \Lambda]\Theta$$

$$[\Lambda\Omega, \Theta] = \Lambda[\Omega, \Theta] + [\Lambda, \Theta]\Omega$$

Also note

IDENTITY OPERATOR

$$\Omega^{-1}\Omega = \Omega\Omega^{-1} = \mathbb{1}$$

$$\Downarrow$$

$$(\Omega\Lambda)^{-1} = \Lambda^{-1}\Omega^{-1}$$

Matrix representation of linear operators in $\mathbb{V}^n$

$$|V\rangle \rightarrow \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} \langle 1|V\rangle \\ \langle 2|V\rangle \\ \vdots \\ \langle n|V\rangle \end{pmatrix}$$

$$\Omega \rightarrow \begin{array}{c} \begin{array}{cccc} \Omega_{11} & \Omega_{12} & & \Omega_{1n} \end{array} \\ \begin{pmatrix} \langle 1|\Omega|1\rangle & \langle 1|\Omega|2\rangle & \cdots & \langle 1|\Omega|n\rangle \\ \langle 2|\Omega|1\rangle & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \langle n|\Omega|1\rangle & & & \langle n|\Omega|n\rangle \end{pmatrix} \end{array}$$

- $$\langle j|\underbrace{\Omega|i\rangle}_{|i'\rangle} = \langle j|i'\rangle \equiv \Omega_{ji}$$

n^2 MATRIX ELEMENTS!

- Examples: 1) the <u>identity operator</u> $\mathbb{1}$

2) the <u>projection operator</u> $\mathbb{P}_i = |i\rangle\langle i|$

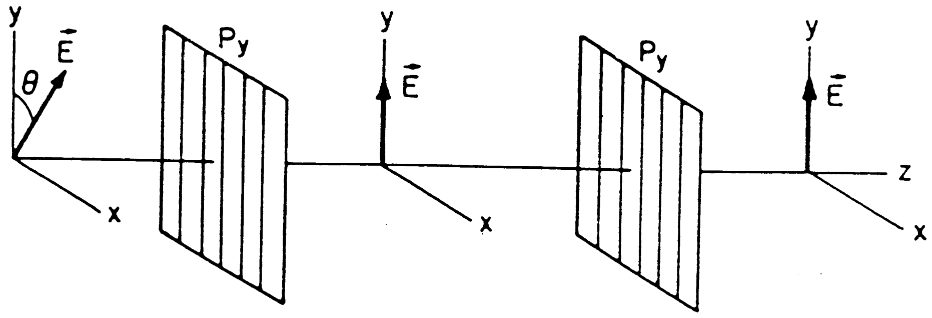
projects out the component of a vector along $|i\rangle$

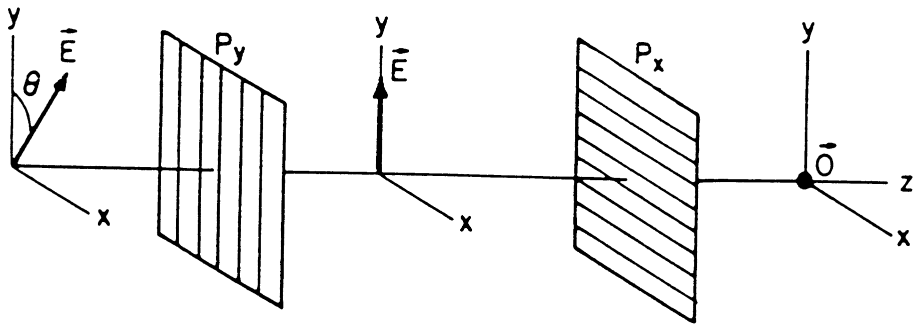
- RESOLUTION OF THE IDENTITY

$$\mathbb{1} = \sum_{i=1}^{n} |i\rangle\langle i| = \sum_{i=1}^{n} \mathbb{P}_i$$

cf. optical polarizers!

$$\mathbb{P}_i \mathbb{P}_j = |i\rangle\langle i|j\rangle\langle j| = \delta_{ij}\,|i\rangle\langle j| = \delta_{ij}\,\mathbb{P}_j$$





Matrix elements of the projection operator

$$(\mathbb{P}_i)_{kl} = \langle k|\mathbb{P}_i|l\rangle = \langle k|i\rangle\langle i|l\rangle = \delta_{ki}\delta_{il}$$

ONE MORE IMPORTANT EXAMPLE : SPIN OPERATORS

(see Sakurai)

- Products of operators $(\Omega\Lambda)_{ij} = \sum_k \Omega_{ik}\Lambda_{kj}$.

Adjoint of an operator

$$\Omega|V\rangle = |\Omega V\rangle \xleftrightarrow{\text{DC}} \langle\Omega V| = \langle V|\Omega^{+}$$

ADJOINT OF Ω.

$$(\Omega^{+})_{ij} = \langle i|\Omega^{+}|j\rangle = \langle\Omega i|j\rangle = \langle j|\Omega i\rangle^{*}$$

$$= \langle j|\Omega|i\rangle^{*} = (\Omega)^{*}_{ji}$$

<u>Taking the adjoint of an equation:</u>

Reverse the order of all factors and make the replacements

$$|\ \rangle \longleftrightarrow \langle\ |$$

$$\Omega \longleftrightarrow \Omega^{+}$$

$$\alpha \longleftrightarrow \alpha^{*}$$

NOTE $\quad (\Omega\Lambda)^{+} = \Lambda^{+}\Omega^{+}$

- <u>Def.</u> Hermitian operator: $\Omega^{+} = \Omega$

<u>Def.</u> anti-Hermitian operator : $\Omega^{+} = -\Omega$

<u>Def.</u> Unitary operator : $U U^{+} = \mathbb{1} \Rightarrow U^{+} = U^{-1}$

$$\Downarrow$$

<u>Theorem</u> Unitary operators preserve inner products

Unitary operators are generalizations of "rotation operators"

<u>Theorem</u> The columns (or rows) of a unitary matrix U form an ON basis in the (sub)space in which U acts.

$$U \longrightarrow \begin{pmatrix} \langle 1|U|1\rangle & \langle 1|U|2\rangle & \cdots & \langle 1|U|n\rangle \\ \langle 2|U|1\rangle & \cdots & & \vdots \\ \vdots & & \ddots & \vdots \\ \langle n|U|1\rangle & \cdots & & \langle n|U|n\rangle \end{pmatrix}$$

The eigenvalue problem

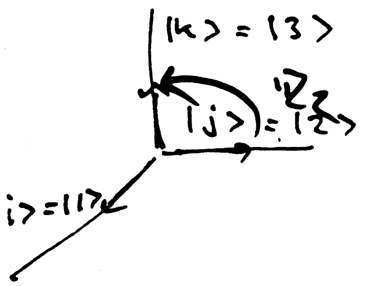
Eigenkets $|V\rangle$ to Ω : $\Omega|V\rangle = \underset{\text{EIGENVALUE}}{\omega}\,\underset{\text{EIGENKETS}}{|V\rangle}$

Example: the <u>projection operator</u> $\Omega = \mathbb{P}_V = |V\rangle\langle V|$

EIGENKETS $\{\alpha|V\rangle\}$, EIGENVALUE $= 1$

Another example: a <u>rotation operator</u> in $V^3(C)$

$$\Omega = R\left(\tfrac{\pi}{2}\mathbf{i}\right) \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$



$$\Omega|1\rangle = |1\rangle$$
$$\Omega|2\rangle = |3\rangle$$
$$\Omega|3\rangle = -|2\rangle$$

that's it? No, there are two more!

!

The characteristic equation $\qquad |v\rangle \in V^n$

$$\Omega|V\rangle = \omega|V\rangle \Rightarrow (\Omega - \omega \mathbb{1})|V\rangle = 0$$

$\Downarrow$ CONDITION FOR NON-ZERO EIGENVALUES

$$\det(\Omega - \omega\mathbb{1}) = 0$$

$$\Downarrow$$

$$\sum_{m=0}^{n} c_m \omega^m = 0 \qquad \text{CHARACTERISTIC EQUATION}$$

$$P^n(\omega) = \sum_{m=0}^{n} c_m \omega^m$$

characteristic polynomial $\longrightarrow$ **with n zeroes**

$\Rightarrow$ **every operator in** V^n **has n eigenvalues**

Check: our rotation operator in $V^3(C)$ **!**

$$\Omega = R\left(\tfrac{\pi}{2}\mathbf{i}\right) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \det(R - \omega\mathbb{1}) = \begin{vmatrix} 1-\omega & 0 & 0 \\ 0 & -\omega & -1 \\ 0 & 1 & \omega \end{vmatrix}$$

CHARACTERISTIC EQUATION : $(1-\omega)(\omega^2+1) = 0 \Rightarrow \omega = 1, \pm i$

EIGENVECTORS $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}$

If the spectrum is *non-degenerate* the eigenvalues can be used to label the eigenvectors

$$\Omega|\omega\rangle = \omega|\omega\rangle$$

Theorem The eigenvalues of a Hermitian operator are real

Theorem To every Hermitian operator Ω there exists (at least) a basis consisting of its ON eigenvectors. Ω is diagonal in this basis and has its eigenvalues as its diagonal elements.

Theorem The *eigenvalues* of a unitary operator are complex numbers of "unit modulus"

Theorem The *eigenvectors* of a unitary operator are mutually orthogonal (assuming no degeneracy).

Diagonalization of Hermitian operators:

Every Hermitian operator on $V^n(\mathbb{C})$ *can be diagonalized by a unitary change of basis*

Simultaneous diagonalization of two Hermitian operators:

Theorem $[\Omega, \Lambda] = 0 \Rightarrow$ there exists (at least) a basis of common eigenvectors that diagonalizes both Ω and Λ

Simple proof if at least one of the operators is non-degenerate.

What if both operators are degenerate? The theorem is still OK but the eigenbasis is not necessarily unique. In general, for finite-dimensional vector spaces we can always find additional operators that commute with each other and together nail down a unique, common eigenbasis. In QUANTUM MECHANICS we assume that such a *complete set of commuting operators* (which together nail down a unique, common eigenbasis) exists also if the vector space is infinite-dimensional.

The "postulates" of (non-relativistic) quantum mechanics

Classical mechanics

I.

The state of a particle at any given time is specified by the two variables x(t) and p(t), i.e. as a point in a two-dimensional phase space.

II.

Every dynamical variable ω is a function of x and p: $\omega = \omega(x,p)$.

We need a [illegible] extension

III.

If the particle is in a state given by x and p, the measurement of the variable ω will yield a value $\omega(x,p)$. The state will remain unaffected.

IV.

CLASSICAL TIME EVOLUTION

Quantum mechanics

I.

The state of the particle is represented by a vector $|\psi(t)\rangle$ in a Hilbert space.

II.

The independent variables x and p of classical mechanics are represented by Hermitian operators X and P with the following matrix elements in the eigenbasis of X:

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

$$\langle x|P|x'\rangle = -i\hbar\,\delta'(x-x')$$

The operators corresponding to dependent variables $\omega(x,p)$ are Hermitian operators

$$\Omega(X,P) = \omega(x \to X, p \to P)$$

III.

If the particle is in a state $|\psi\rangle$, a measurement of the variable (corresponding to) Ω will yield one of the eigenvalues ω, with probability $P(\omega) \sim |\langle\omega|\psi\rangle|^2$. The state of the system will change from $|\psi\rangle$ to $|\omega\rangle$ as a result of the measurement.

IV.

QUANTUM TIME EVOLUTION

(LATER)

Possible oucomes of an experiment measuring ω ?

Classically

Parrticle in a state $(x, p) \longrightarrow \omega(x, p)$

Quantum

Particle in a state $|\psi(t)\rangle$

four-step program *(← postulates I - III)*

<u>step 1</u>: construct $\Omega = \omega(x \to X, p \to P)$

<u>step 2</u>: find the eigenkets $|\omega_i\rangle$ and eigenvalues ω_i of Ω

<u>step 3</u>: expand $|\psi\rangle$ in this basis :

$$|\psi\rangle = \sum_{i=1}^{n} |\omega_i\rangle\langle\omega_i|\psi\rangle$$

<u>step 4</u>: the probability $P(\omega_i)$ of measuring ω_i :

$$P(\omega_i) \sim |\langle\omega_i|\psi\rangle|^2 = \langle\psi|\omega_i\rangle\langle\omega_i|\psi\rangle$$

$$= \langle\psi|\mathbb{P}_{\omega_i}|\psi\rangle$$