

Fundamental Concepts and Dirac Formalism in Quantum Mechanics¹

The Dirac formalism is a general and abstract formulation of quantum mechanics (QM), which includes wave mechanics and matrix mechanics as special cases. The value of the wave function in a point, $\psi(x)$, or the elements a_i in a column matrix, can be seen as *coordinates* for an abstract *vector* Ψ , which contains *all information* about the state of the system.

**A physical state is represented by a state vector
in a complex linear vector space in N dimensions.**

Dimension = the number (#) of possible results of a measurement of the dynamical variables that characterize the system, e.g. $N = 2$ for spin of spin-1/2 particle, $N = \infty$ (non-denumerable, Hilbert space) for position of particle in space.

Notation: "ket" $|\alpha\rangle$ (α specifies the state, e.g. spin, position etc, c.f. ψ_α)

Sum: $|\alpha\rangle + |\beta\rangle = |\gamma\rangle$, i.e. a ket vector

Multiplication with complex number: $c|\alpha\rangle = |\alpha\rangle c = |\gamma'\rangle$, i.e. a ket

Postulate: $|\alpha\rangle$ and $c|\alpha\rangle$ represent the *same* physical state, i.e. the "direction" contains information but not the "normalisation".

Scalar (inner) product

In wave/matrix mechanics "order" matters, e.g. $(\psi_\beta, \psi_\alpha) = \int dx \psi_\beta^*(x)\psi_\alpha(x) = (\psi_\alpha, \psi_\beta)$

In a complex linear vector space one must distinguish "prefactors" and "postfactors".

The scalar product is antilinear and linear with respect to these.

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

Anti-linear operator: $A(c_1\psi_1 + c_2\psi_2) = c_1^* A\psi_1 + c_2^* A\psi_2$

Let pre- and postfactors be vectors in two *different complex linear vector spaces*; which are anti-linearly related: **ket space** with ket vectors $|\alpha\rangle$, **bra space** with bra vectors $\langle\alpha|$

There is a unique anti-linear **dual correspondence** (DC) between these vector spaces:

$|\alpha\rangle \longleftrightarrow \langle\beta|$ (note, same α) and $c_\alpha |\alpha\rangle + c_\beta |\beta\rangle \longleftrightarrow c_\alpha^* \langle\alpha| + c_\beta^* \langle\beta|$.

Scalar (or inner) product: $\langle\beta|\alpha\rangle$ (i.e. "bra-c-ket") is a complex number $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$

Norm $\|\alpha\|^2 = \langle\alpha|\alpha\rangle = \langle\alpha|\alpha\rangle^*$ is real

Postulate: positive definite metric $\|\alpha\|^2 = \langle\alpha|\alpha\rangle \geq 0$

Normalized vector $|\hat{\alpha}\rangle = |\alpha\rangle/\sqrt{\langle\alpha|\alpha\rangle}$

$|\alpha\rangle$ and $|\beta\rangle$ **orthogonal** if $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* = 0$

¹Lecture notes on Quantum Mechanics, advanced course at Uppsala University, corresponding to 1st chapter of J.J. Sakurai, Modern Quantum Mechanics

Operators (\supset observables)

Operator X acting from left/right on ket/bra gives new ket/bra: $X|\alpha\rangle = |\alpha'\rangle$, $\langle\beta|X = \langle\beta'|$

$X = Y$ iff (=if and only if) $X|\alpha\rangle = Y|\alpha\rangle$ for arbitrary (*i.e.* all) $|\alpha\rangle$

Hermitian conjugate X^\dagger defined through the dual correspondence $X|\alpha\rangle \longleftrightarrow \langle\alpha|X^\dagger$

Hermitian operator $X = X^\dagger$, *i.e.* $X|\alpha\rangle \longleftrightarrow \langle\alpha|X$

c.f. Hermitian conjugate in wave mechanics $\int dx \psi_\beta^*(x) X \psi_\alpha(x) = \int dx (X^\dagger \psi_\beta(x))^* \psi_\alpha(x)$ (1)

Addition: (a) $X + Y = Y + X$ commutative

(b) $X + (Y + Z) = (X + Y) + Z$ associative

Multiplication: (a) $XY \neq YX$ non-commutative in general

(b) $X(YZ) = (XY)Z$ associative \leftarrow postulate/axiom

(c) $(XY)^\dagger = Y^\dagger X^\dagger$

In Dirac (1) becomes $\langle\beta|(X|\alpha\rangle) \stackrel{(b)}{=} (\langle\beta|X)|\alpha\rangle \stackrel{def.}{=} \langle\beta|X|\alpha\rangle$, which is a complex number (c-#).

Hence $\langle\beta|X|\alpha\rangle = \langle\beta|(X|\alpha\rangle) \stackrel{(c), DC}{=} \{(\langle\alpha|X^\dagger)|\beta\rangle\}^* = \langle\alpha|X^\dagger|\beta\rangle^*$ (see (1.2.38-39) in Sakurai)

Therefore X Hermitian $\Leftrightarrow \langle\beta|X|\alpha\rangle = \langle\alpha|X|\beta\rangle^*$

The associative axiom also gives $(|\beta\rangle\langle\alpha|)|\gamma\rangle = |\beta\rangle(\langle\alpha|\gamma\rangle) \equiv |\beta\rangle\langle\alpha|\gamma\rangle$. Here, $|\beta\rangle\langle\alpha|$ can be seen as an *operator* acting on ket $|\gamma\rangle$ giving new ket vector in *direction* $|\beta\rangle$.

Observables

Theorem: (in linear algebra) The eigenvalues to a Hermitian operator are real, the eigenvectors corresponding to different eigenvalues are orthogonal. (Proof: Sakurai p. 17.)

Every physical, measurable quantity (dynamical variable) is represented by an operator (acting on ket space) with specific properties, *e.g.* real eigenvalues and expectation values, and must hence be Hermitian. Called *observable*, denoted $A, B, C \dots$

A ket is an **eigenvector** (eigenstate) to A if $A|a'\rangle = a'|a'\rangle$, where a' is an **eigenvalue** to A .

A has eigenvalues $a', a'' \dots$, *i.e.* $A|a'\rangle = a'|a'\rangle$, $A|a''\rangle = a''|a''\rangle$, \dots

One uses *orthonormal* eigenvectors to observable A , *i.e.* $\langle a'|a''\rangle = \delta_{a'a''}$

Postulate: the set of eigenvectors $\{|a^{(i)}\rangle\}$ to an observable A constitute a **complete basis** in ket space.

Thus, every state vector $|\alpha\rangle$ can be expanded in the eigenvectors to a Hermitian observable A

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle \text{ or } \sum_i c_i |a^{(i)}\rangle \text{ (superposition principle)}$$

The ket space is "spanned" by the eigenvectors. The expansion coefficients c_i are obtained from

$$\langle a^{(j)}|\alpha\rangle = \sum_i c_i \langle a^{(j)}|a^{(i)}\rangle = c_j \Rightarrow \boxed{c_i = \langle a^{(i)}|\alpha\rangle}$$

i.e. the scalar products with the basis vectors (*c.f.* an ordinary vector $\vec{v} = \hat{x}(\hat{x}\cdot\vec{v}) + \hat{y}(\hat{y}\cdot\vec{v}) + \hat{z}(\hat{z}\cdot\vec{v})$).

Hence, one can write $|\alpha\rangle = \sum_i |a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle$, where $\langle a^{(i)}|\alpha\rangle$ are the coordinates in the basis $\{|a^{(i)}\rangle\}$.

Here, $\sum_i |a^{(i)}\rangle \langle a^{(i)}|$ can be seen as an operator acting on $|\alpha\rangle$, and since $|\alpha\rangle$ is arbitrary one obtains

$$\boxed{\sum_i |a^{(i)}\rangle \langle a^{(i)}| = 1} \text{ which is the } \mathbf{completeness relation}, \text{ very useful!!!}$$

Example: $\|\alpha\|^2 = \langle\alpha|\alpha\rangle = \langle\alpha|\sum_i |a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle = \sum_i \langle\alpha|a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle = [\text{using } \langle a^{(i)}|\alpha\rangle = \langle\alpha|a^{(i)}\rangle^*]$
 $= \sum_i |\langle\alpha|a^{(i)}\rangle|^2 = \sum_i |c_i|^2$

Projection operators: $(|a^{(i)}\rangle \langle a^{(i)}|)|\alpha\rangle = c_i |a^{(i)}\rangle$, *i.e.* the component of $|\alpha\rangle$ in direction $|a^{(i)}\rangle$.

Let $\Lambda_i = |a^{(i)}\rangle \langle a^{(i)}|$ and the completeness relation can also be written $\sum_i \Lambda_i = 1$

Matrix representations

Complex linear vector space, vectors $|\alpha\rangle$

Basis: eigenvectors $|a^{(i)}\rangle$ to observable A , *i.e.* $|\alpha\rangle = \sum_i |a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle$ where $c_i = \langle a^{(i)}|\alpha\rangle$ are the coordinates in this basis.

The ket vector's coordinate representations in different bases relates the Dirac state vector to Heisenberg's matrix algebra or Schrödinger's wave mechanics.

The Dirac state vector is **represented by** (\doteq) a column matrix (vector)

$$|a^{(1)}\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, |a^{(2)}\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \dots ; |\alpha\rangle \doteq \begin{pmatrix} \langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \langle a^{(3)}|\alpha\rangle \\ \vdots \end{pmatrix}$$

The state vector is thus represented by its coordinates in different bases. These coordinates depend on the chosen basis, but for any basis they provide *complete information on the state*.

$$\text{An operator } X \text{ is represented by a matrix: } |\gamma\rangle = X|\alpha\rangle \longleftrightarrow \begin{pmatrix} - \\ - \\ \vdots \end{pmatrix} = \begin{pmatrix} - & - & \dots \\ - & - & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} - \\ - \\ \vdots \end{pmatrix}$$

The coordinate in direction $|a^{(i)}\rangle$ is $\langle a^{(i)}|\gamma\rangle = \langle a^{(i)}|X|\alpha\rangle = \sum_j \langle a^{(i)}|X|a^{(j)}\rangle \langle a^{(j)}|\alpha\rangle$ which can be interpreted as matrix multiplication with $\langle a^{(i)}|X|a^{(j)}\rangle$ a **matrix element** with index i (j) running over rows (columns):

$$X \doteq \begin{pmatrix} \langle a^{(1)}|X|a^{(1)}\rangle & \langle a^{(1)}|X|a^{(2)}\rangle & \dots \\ \langle a^{(2)}|X|a^{(1)}\rangle & \langle a^{(2)}|X|a^{(2)}\rangle & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

A bra vector, $\langle\beta| = \sum_i \langle\beta|a^{(i)}\rangle \langle a^{(i)}|$, is represented by a conjugated row matrix

$$\langle\beta| = (\langle\beta|a^{(1)}\rangle, \langle\beta|a^{(2)}\rangle, \dots) = (\langle a^{(1)}|\beta\rangle^*, \langle a^{(2)}|\beta\rangle^*, \dots)$$

The inner product $\langle\beta|\alpha\rangle = (-, -, \dots) \begin{pmatrix} - \\ - \\ \vdots \end{pmatrix} = \text{complex number}$.

The outer product gives a matrix, *i.e.* an operator $|\beta\rangle\langle\alpha| = \sum_i \sum_j |a^{(i)}\rangle \langle a^{(i)}|\beta\rangle \langle\alpha|a^{(j)}\rangle \langle a^{(j)}| \doteq$

$$\begin{pmatrix} \langle a^{(1)}|\beta\rangle \langle a^{(1)}|\alpha\rangle^* & \langle a^{(1)}|\beta\rangle \langle a^{(2)}|\alpha\rangle^* & \dots \\ \langle a^{(2)}|\beta\rangle \langle a^{(1)}|\alpha\rangle^* & \langle a^{(2)}|\beta\rangle \langle a^{(2)}|\alpha\rangle^* & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} \langle a^{(1)}|\beta\rangle \\ \langle a^{(2)}|\beta\rangle \\ \vdots \end{pmatrix} (\langle a^{(1)}|\alpha\rangle^*, \langle a^{(2)}|\alpha\rangle^*, \dots)$$

An observable A is represented by a *diagonal* matrix in its own eigenvector system $\langle a^{(i)}|A|a^{(j)}\rangle =$

$$a^{(j)} \langle a^{(i)}|a^{(j)}\rangle = a^{(j)} \delta_{ij} \Rightarrow A \doteq \begin{pmatrix} a^{(1)} & 0 & \dots \\ 0 & a^{(2)} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

This gives, *e.g.*, $A = \sum_i \sum_j |a^{(i)}\rangle \langle a^{(i)}|A|a^{(j)}\rangle \langle a^{(j)}| = \sum_i a^{(i)} |a^{(i)}\rangle \langle a^{(i)}| = \sum_i a^{(i)} \Lambda_i$

Observable and eigenvalues \longleftrightarrow physical measuring process

Measurement of a physical variable corresponding to observable A gives the eigenvalues of A as the only possible results.

- discrete eigenvalue spectrum: measurement gives $a^{(i)}, i = 1, 2, \dots$ (quantization)
- probability for outcome $a^{(i)}$ given by the (normalized) state $|\alpha\rangle$ before measurement:
 $|\alpha\rangle = \sum_i |a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle \xrightarrow{\text{postulate}} \text{probability} = |\langle a^{(i)}|\alpha\rangle|^2 = |c_i|^2$
- measuring process changes the state, which goes into an eigenstate of A :
 $|\alpha\rangle \xrightarrow{A\text{-measurement}} |a^{(i)}\rangle$ the wave function "collapses" (unless $|\alpha\rangle$ already = $|a^{(i)}\rangle$)

Determination of probabilities $|\langle a^{(i)}|\alpha\rangle|^2$ require many measurements on *identical systems*, *i.e.* prepared in state $|\alpha\rangle$ ("ensemble").

Definition: the **expectation value** of A with respect to state $|\alpha\rangle$ is the mean value of the results of many measurements: $\langle A \rangle \equiv \langle \alpha|A|\alpha\rangle = \sum_i \sum_j \langle \alpha|a^{(i)}\rangle \langle a^{(i)}|A|a^{(j)}\rangle \langle a^{(j)}|\alpha\rangle = \sum_i a^{(i)} |\langle a^{(i)}|\alpha\rangle|^2$

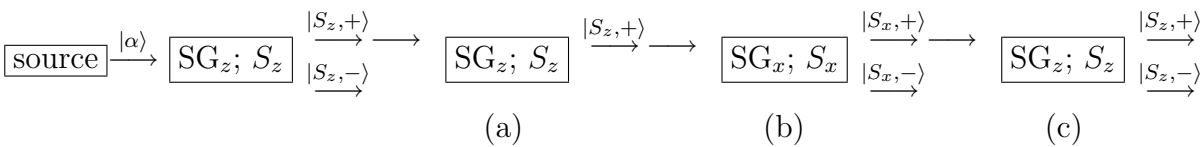
- the eigenvalues $a^{(i)}$ are independent of $|\alpha\rangle$, $|\alpha\rangle$ gives probability for outcome $a^{(i)}$
- distinguish eigenvalue and expectation value, the expectation value is a weighted sum of eigenvalues and is not quantized

Example: Stern-Gerlach measurement of spin 1/2 system

Measuring the spin along a quantization axis, *e.g.* z , corresponds to applying the operator S_z

$$|\alpha\rangle \xrightarrow{S_z} \begin{cases} |S_z, +\rangle = |+\hbar/2\rangle \\ |S_z, -\rangle = |-\hbar/2\rangle \end{cases} \text{ with probability } \begin{cases} |\langle S_z, +|\alpha\rangle|^2 \\ |\langle S_z, -|\alpha\rangle|^2 \end{cases}$$

A source gives spin 1/2 "particles" (*e.g.* electrons or atoms with total angular momentum 1/2), giving the initial state $|\alpha\rangle$ which can be expanded in eigenfunctions to the observable S_z as $|\alpha\rangle = c_+|S_z, +\rangle + c_-|S_z, -\rangle$. The beam of particles pass a Stern-Gerlach magnet (SG), which splits it into the two eigenstates of the corresponding spin operator (*e.g.* S_z). One of the emerging beams can then be blocked and the other goes into another Stern-Gerlach magnet:



- repeated measurement of S_z gives $|S_z, +\rangle$ with probability =1.
- measurement of new variable S_x gives two possible outcomes $|S_x, +\rangle$ or $|S_x, -\rangle$ with probability 1/2 each. The state is changed and the information on S_z is destroyed.
- measurement of new variable S_z gives $|S_z, +\rangle$ or $|S_z, -\rangle$ with probability 1/2 each. The state is changed again and the information on S_x is destroyed.

One *cannot have simultaneous information* about the x and z components of the spin. S_x and S_z are incompatible observables.

Compatible observables: $[A, B] = AB - BA = 0$ simultaneous measurable with arbitrary accuracy
 Incompatible observables: $[A, B] \neq 0$ not simultaneous measurable with arbitrary accuracy

Theorem: $[A, B] = 0 \Rightarrow A$ and B have common eigenvector system, *i.e.* common basis.

Proof: $B|a^{(i)}\rangle = \sum_j \sum_k |a^{(j)}\rangle \langle a^{(j)}|B|a^{(k)}\rangle \langle a^{(k)}|a^{(i)}\rangle = |a^{(i)}\rangle \langle a^{(i)}|B|a^{(i)}\rangle = b^{(i)}|a^{(i)}\rangle$ *i.e.* $|a^{(i)}\rangle$ is an eigenvector to B with eigenvalue $b^{(i)} = \langle a^{(i)}|B|a^{(i)}\rangle$. The derivation used $\langle a^{(k)}|a^{(i)}\rangle = \delta_{ki}$ and $\langle a^{(j)}|B|a^{(k)}\rangle = 0$ if $a^{(j)} \neq a^{(k)}$ which follows from $[A, B] = 0$ giving $0 = \langle a^{(j)}|[A, B]|a^{(k)}\rangle = (a^{(j)} - a^{(k)})\langle a^{(j)}|B|a^{(k)}\rangle$ (see further Sakurai p. 30).

Let $|a', b'\rangle$ be eigenket to A and B , *i.e.* $A|a', b'\rangle = a'|a', b'\rangle$ and $B|a', b'\rangle = b'|a', b'\rangle$

$$|\alpha\rangle \xrightarrow{1: \text{measure } A} |a', b'\rangle \xrightarrow{2: \text{measure } B} |a', b'\rangle \xrightarrow{3: \text{measure } A} |a', b'\rangle$$

1. Measure $A \longrightarrow$ result: a' and eigenstate $|a', b'\rangle$
2. Measure $B \longrightarrow$ result: b' with probability 1 and eigenstate $|a', b'\rangle$ (unchanged)
3. Measure $A \longrightarrow$ result: a' with probability 1 and eigenstate $|a', b'\rangle$ (unchanged)

System in state where A and B exactly measurable simultaneously. The observables do not affect each other.

Example: Orbital angular momentum operators \vec{L}^2 and L_z with eigenvectors $|\ell, m_z\rangle$.

Degeneration: two or more linearly independent eigenkets to A with the same eigenvalue.

A complete set of commuting observables $A, B, C \dots$ lifts the degeneration completely and the common eigenvectors $|a', b', c' \dots\rangle$, which are uniquely determined by the quantum numbers $a', b', c' \dots$, defines a *basis*.

Theorem: If $[A, B] \neq 0$, then A and B cannot have a complete set of common eigenvectors. (Proof: see Sakurai p. 32)

Subspace with common eigenvectors may exist, *e.g.* $|\ell = 0, m_z = 0\rangle$ is common eigenvector to \vec{L}^2, L_z and L_x, L_y .

Dispersion = variance = mean square deviation of A is

$$\langle(\Delta A)^2\rangle = \langle(A - \langle A\rangle)^2\rangle = \langle(A^2 - 2A\langle A\rangle + \langle A\rangle^2)\rangle \equiv \langle A^2\rangle - \langle A\rangle^2$$

and specifies the "uncertainty" of the variable corresponding to operator (measurement) A .

Since $\langle \dots \rangle = \langle \alpha | \dots | \alpha \rangle$, $\langle(\Delta A)^2\rangle = 0$ for an eigenstate ($|\alpha\rangle = |a'\rangle$) to A .

Uncertainty relation (derivation Sakurai p. 35-36) $\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4} |\langle[A, B]\rangle|^2$ (2)

Note: coefficient 1/4 exactly specified. This is generalisation of Heisenberg's uncertainty relation for x and p (and E, t).

If $[A, B] \neq 0$, then A and B cannot be determined exactly simultaneously — the measurements corresponding to A and B affect each other.

If system is an eigenstate to A , then $\langle(\Delta A)^2\rangle = 0 \Rightarrow \langle(\Delta B)^2\rangle \rightarrow \infty$, *i.e.* B is totally undetermined.

Change of basis

Different bases, given by the eigenvectors to different incompatible complete sets of observables, gives different coordinate representations of arbitrary state vector $|\alpha\rangle$. The coordinates in different bases are called different **representations** of $|\alpha\rangle$.

Example: Energy representation $|\alpha\rangle \doteq \begin{pmatrix} \langle E_1|\alpha\rangle \\ \langle E_2|\alpha\rangle \\ \vdots \end{pmatrix}$ or position representation $\psi_\alpha(x) \equiv \langle x|\alpha\rangle$.

Simple to change basis in Dirac formalism

Two incompatible observables A and B with complete basis systems $\{|a^{(i)}\rangle\}$ and $\{|b^{(i)}\rangle\}$ are related via a transformation operator U , $|b^{(j)}\rangle = U|a^{(j)}\rangle = \sum_i |a^{(i)}\rangle \langle a^{(i)}|U|a^{(j)}\rangle$ where $i, j = 1, 2, \dots$

The transformation matrix has elements $U^{ij} = \langle a^{(i)}|U|a^{(j)}\rangle = \langle a^{(i)}|b^{(j)}\rangle$, *i.e.* given by the scalar products of the bases.

If orthonormal bases $UU^\dagger = \sum_i U|a^{(i)}\rangle \langle a^{(i)}|U^\dagger = \sum_i |b^{(i)}\rangle \langle b^{(i)}| = 1$, *i.e.* $U^\dagger = U^{-1} \Rightarrow U$ is a **unitary** operator which conserves the norm of states: $|\beta\rangle = U|\alpha\rangle \Rightarrow \langle \beta|\beta\rangle = \langle \alpha|U^\dagger U|\alpha\rangle = \langle \alpha|\alpha\rangle$.

Transformation of the coordinates for $|\alpha\rangle$: $\langle b^{(j)}|\alpha\rangle = \sum_i \langle b^{(j)}|a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle = \sum_i \langle a^{(j)}|U^\dagger|a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle = \sum_i (U^{-1})^{ji} \langle a^{(i)}|\alpha\rangle$. Varying j gives the matrix equation

$$\begin{pmatrix} \vdots \\ \langle b^{(j)}|\alpha\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots & \vdots & \vdots \\ \cdots & (U^{-1})^{ji} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \langle a^{(i)}|\alpha\rangle \\ \vdots \end{pmatrix}$$

Physically: if the probability distribution in one variable (A) is known, one can obtain the probability distribution in an arbitrary (=any) variable (B). Not surprising since $|\alpha\rangle$ contains the complete information about the system.

The matrix elements of arbitrary operator is transformed according to $\langle b^{(j)}|X|b^{(i)}\rangle = \sum_m \sum_n \langle b^{(j)}|a^{(m)}\rangle \langle a^{(m)}|X|a^{(n)}\rangle \langle a^{(n)}|b^{(i)}\rangle = \sum_m \sum_n \langle a^{(j)}|U^\dagger|a^{(m)}\rangle \langle a^{(m)}|X|a^{(n)}\rangle \langle a^{(n)}|U|a^{(i)}\rangle$, *i.e.* $(X')^{ji} = (U^\dagger)^{jm} X^{mn} U^{ni}$. Varying j, i gives the matrix equation $X' = U^\dagger X U$, where X' is in the $\{|b^{(j)}\rangle\}$ basis and X in the $\{|a^{(j)}\rangle\}$ basis. This is a similarity transformation of a matrix as in linear algebra.

Trace of an operator is the sum of the diagonal elements $tr(X) = \sum_i \langle a^{(i)}|X|a^{(i)}\rangle$, which is conserved in a unitary transformation.

Continuous eigenvalue spectra

For example position, momentum etc. (but also energy etc is not always quantized).

Eigenvalue equation: $\xi|\xi'\rangle = \xi'|\xi'\rangle$ where ξ is the position operator and ξ' is its eigenvalue giving the position in ordinary space of the system (*e.g.* a particle).

Use above formalism for discrete spectra with replacements: $\sum_i \longrightarrow \int d\xi'$ and $\delta_{ij} \longrightarrow \delta(\xi' - \xi'')$

Giving: $\langle a^{(i)}|a^{(i)}\rangle = \delta_{ij} \longrightarrow \langle \xi'|\xi''\rangle = \delta(\xi' - \xi'')$
 $\sum_i |a^{(i)}\rangle \langle a^{(i)}| = 1 \longrightarrow \int d\xi' |\xi'\rangle \langle \xi'| = 1$ completeness relation
 $|\alpha\rangle = \sum_i |a^{(i)}\rangle \langle a^{(i)}|\alpha\rangle \longrightarrow |\alpha\rangle = \int d\xi' |\xi'\rangle \langle \xi'|\alpha\rangle$ expansion in eigenvectors

Position representation and position measurement

Consider first one dimension x . **Position operator** $x|x'\rangle = x'|x'\rangle$

Postulate: eigenvectors of position operator constitute a complete basis.

Thus, an arbitrary state vector can be expanded as $|\alpha\rangle = \int_{x'_{min}}^{x'_{max}} dx' |x'\rangle \langle x'|\alpha\rangle$ with expansion coefficient $c_{x'} = \langle x'|\alpha\rangle$ and $|\langle x'|\alpha\rangle|^2 dx' =$ probability to find particle in $[x', x' + dx']$

Normalisation $\langle \alpha|\alpha\rangle = 1 \Rightarrow \int_{x'_{min}}^{x'_{max}} dx' \langle \alpha|x'\rangle \langle x'|\alpha\rangle = 1$, *i.e.* probability=1 to find particle somewhere in available x' -interval.

The state vector's expansion coefficients in position space is the **wave function** $\langle x'|\alpha\rangle = \psi_\alpha(x')$

Scalar product $\langle \beta|\alpha\rangle = \int dx' \langle \beta|x'\rangle \langle x'|\alpha\rangle \stackrel{\langle \beta|x'\rangle = \langle x'|\beta\rangle^*}{=} \int dx' \psi_\beta^*(x') \psi_\alpha(x')$, "overlap integral" giving the probability to find state $|\alpha\rangle$ in state $|\beta\rangle$, or vice versa.

The position operator is, in its own basis, represented by a diagonal "matrix" $\langle x''|x|x'\rangle = x' \langle x''|x'\rangle = x' \delta(x'' - x')$

General operator $f(x)$: $\langle x''|f(x)|x'\rangle = f(x') \delta(x'' - x')$

Expectation value: $\langle \beta|A|\alpha\rangle = \int dx' \int dx'' \langle \beta|x''\rangle \langle x'|A|x''\rangle \langle x''|\alpha\rangle = \int dx' \int dx'' \psi_\beta^*(x'') \langle x'|A|x''\rangle \psi_\alpha(x')$

Spec. for $A = f(x)$: $\langle \beta|f(x)|\alpha\rangle = \int dx' \int dx'' \langle \beta|x''\rangle \langle x'|f(x)|x''\rangle \langle x''|\alpha\rangle = \int dx' \psi_\beta^*(x') f(x') \psi_\alpha(x')$

Generalisation to 3-dim: $|\vec{x}'\rangle = |x', y', z'\rangle$ simultaneous eigenvector to operators x, y, z

$$x|\vec{x}'\rangle = x'|\vec{x}'\rangle, \quad y|\vec{x}'\rangle = y'|\vec{x}'\rangle, \quad z|\vec{x}'\rangle = z'|\vec{x}'\rangle, \quad \text{i.e.} \quad \vec{x}|\vec{x}'\rangle = \vec{x}'|\vec{x}'\rangle$$

If $[x, y] = [y, z] = [x, z] = 0$, then x, y, z have common eigenvectors.

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

Completeness relation: $\int d\vec{x}' |\vec{x}'\rangle \langle \vec{x}'| = 1$

Expansion in eigenstates: $|\alpha\rangle = \int d\vec{x}' |\vec{x}'\rangle \langle \vec{x}'|\alpha\rangle$, where the expansion coefficient $\langle \vec{x}'|\alpha\rangle = \psi_\alpha(\vec{x}')$ is the wave function in 3 dimensions.

The translation operator: Infinitesimal translation $\mathcal{T}(dx')|x'\rangle = |x' + dx'\rangle$. Properties:

1. conservation of probability \Rightarrow conservation of norm $\Rightarrow \mathcal{T}$ unitary ($\mathcal{T}^\dagger = \mathcal{T}^{-1}$)
 $\langle \alpha|\alpha\rangle = \langle \alpha|\mathcal{T}^\dagger \mathcal{T}|\alpha\rangle$
2. successive translations $\mathcal{T}(dx'')\mathcal{T}(dx')|x'\rangle = \mathcal{T}(dx'')|x'' + dx'\rangle = |x'' + dx' + dx''\rangle = \mathcal{T}(dx'' + dx')|x'\rangle$
3. inverse \Leftrightarrow opposite direction translation $\mathcal{T}^{-1}(dx') = \mathcal{T}(-dx')$
4. $dx' \rightarrow 0$ gives the identity operator, *i.e.* $\lim_{dx' \rightarrow 0} \mathcal{T}(dx') = 1$

A unitary operator can be written $U = e^{iA} \equiv 1 + iA + \frac{(iA)^2}{2!} + \dots$ where A is a Hermitian operator. This gives $U^\dagger U = e^{-iA^\dagger} e^{iA} = e^{-iA} e^{iA} = 1 = e^{iA} e^{-iA} = U U^\dagger$, *i.e.* U is unitary and satisfies condition 1.

A linear in $dx' \Rightarrow 2$ is satisfied. With $\mathcal{T}(dx') = e^{-ikdx'} = 1 - ikdx' + \dots$ condition 3 and 4 OK.

What is k ?

Examine $|\alpha'\rangle = \mathcal{T}(dx')|\alpha\rangle$: $\psi_{\alpha'}(x') = \langle x'|\alpha'\rangle = \langle x'|\mathcal{T}(dx')|\alpha\rangle \stackrel{\text{hint}}{=} \langle x' - dx'|\alpha\rangle = \psi_{\alpha}(x' - dx')$

(hint: $\langle x'|\mathcal{T}(dx') \xrightarrow{DC} \mathcal{T}^\dagger(dx')|x'\rangle = \mathcal{T}^{-1}(dx')|x'\rangle = \mathcal{T}(-dx')|x'\rangle = |x' - dx'\rangle \xrightarrow{DC} \langle x' - dx'|$)

Thus, underlined parts give $\langle x'|1 - ikdx' + \dots|\alpha\rangle = \psi_{\alpha}(x' - dx')$. Using in the left-hand side (LHS) that i and dx' are numbers (not operators) and can be moved out from brackets, and Taylor expanding the right-hand (RHS) gives the equation

$$\langle x'|\alpha\rangle - i\langle x'|k|\alpha\rangle dx' + \dots = \psi_{\alpha}(x') - \frac{d}{dx'}\psi_{\alpha}(x')dx' + \dots$$

Since dx' can be varied, this equation implies that terms of the same order in dx' on both sides have to be equal. Thus, equating the first order terms gives

$$\langle x'|k|\alpha\rangle = -i\frac{d}{dx'}\psi_{\alpha}(x') \quad (= -i\frac{d}{dx'}\langle x'|\alpha\rangle) \quad (3)$$

Sakurai (p. 46) shows $[x, \mathcal{T}(dx')] = dx'$, which gives $[x, k] = i$. Since $[x, p] = i\hbar$ it is reasonable to let $k = p/\hbar = 2\pi/\lambda$ (wave number). This gives

$$\langle \beta|p|\alpha\rangle = \int dx' \langle \beta|x'\rangle \langle x'|\hbar k|\alpha\rangle = \int dx' \psi_{\beta}^*(x') (-i\hbar\frac{d}{dx'})\psi_{\alpha}(x')$$

where eq. (3) has been used in the last step which displays the momentum operator in position space representation: $-i\hbar\frac{d}{dx'}$

The uncertainty relation (2) then specifies exactly $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle \geq \frac{1}{4} |\langle[x, p]\rangle|^2 = \hbar^2/4$

Thus, the momentum operator p is the *generator* for translations in position space and the infinitesimal translation operator is $\mathcal{T}(dx') = 1 - i\frac{p}{\hbar}dx'$

(*c.f.* canonical transformations in classical mechanics, where generalized momentum p generates transformations $q \rightarrow q + dq$ in the corresponding generalized (conjugated) coordinate q .)

Finite translation: $\mathcal{T}(\Delta x') = \lim_{N \rightarrow \infty} (1 - \frac{ip}{\hbar} \frac{\Delta x'}{N})^N = \exp(-\frac{ip}{\hbar} \Delta x')$

Generalisation to 3-dim: $\mathcal{T}(dx') = 1 - i\vec{p} \cdot d\vec{x}'/\hbar$ and $\mathcal{T}(\Delta \vec{x}') = \exp(-\frac{i\vec{p}}{\hbar} \Delta \vec{x}')$

The momentum representation

Dynamical variable $p \longleftrightarrow$ operator p . Basis $p|p'\rangle = p'|p'\rangle$

Vector $|\alpha\rangle = \int dp' |p'\rangle \langle p'|\alpha\rangle$; $|\langle p'|\alpha\rangle|^2 dp' =$ probability $p \in [p', p' + dp']$

Wave function in momentum space $\Phi_{\alpha}(p') = \langle p'|\alpha\rangle$

Coordinates in position and momentum representation related: $\langle x'|\alpha\rangle = \int dp' \underbrace{\langle x'|p'\rangle}_{*} \langle p'|\alpha\rangle$ (4)

* interpreted as transformation "matrix" from $|x'\rangle$ -basis to $|p'\rangle$ -basis

* also wave function for momentum eigenstate $|p'\rangle$

Since $\langle x'|p|p'\rangle = p'\langle x'|p'\rangle$ and, using eq. (3), the LHS can be written $-i\hbar\frac{d}{dx'}\langle x'|p'\rangle$ and one obtains the very simple first order differential equation

$$-i\hbar\frac{d}{dx'}\langle x'|p'\rangle = p'\langle x'|p'\rangle$$

with the solution $\langle x'|p'\rangle = N \exp(ip'x'/\hbar)$, where $N = 1/\sqrt{2\pi\hbar}$ from the normalisation condition. This is the plane wave obtained without solving a second order Schrödinger equation!

Equation (4) can then be written

$$\psi_{\alpha}(x') = N \int dp' e^{ip'x'/\hbar} \Phi_{\alpha}(p')$$

which is the Fourier expansion of $\psi_{\alpha}(x')$ in eigenfunctions $N e^{ip'x'/\hbar}$ to p . The wave function of $|\alpha\rangle$ in p -space is

$$\Phi_{\alpha}(p') = \langle p'|\alpha\rangle = \int dx' \langle p'|x'\rangle \langle x'|\alpha\rangle = N \int dx' e^{-ip'x'/\hbar} \psi_{\alpha}(x')$$

i.e. the Fourier transform is contained in the Dirac formalism.