Notes of Quantum Mechanics

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Preface

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Chapter 1

Mathematical Formalism

1.1 Introduction

The formalism of quantum mechanics (QM) involves symbols and methods for denoting and determining the time dependent state of a physical system along with a mathematical structure for evaluating the possible outcomes and associated proabailities of measurements.

State

A **state** is evything knowable about the dynamical aspects of a system at a certain time.

A particle has associated a **wavefunction** $\psi(\boldsymbol{r},t)$ whose probability interpretation resides on $|\psi(\boldsymbol{r},t)|^2$: it represents the probabilifty density function which serves a a probability finder in space and time. The probability of finding the particle somewhere in space is thus equal to 1:

$$\int_{\text{all space}} d^3r\ |\psi(\boldsymbol{r},t)|^2 = 1. \tag{1.1}$$

Thus, in order that this integral converges, we must deal with a set of square-integrable functions, called L^2. We can only retain the functions $\psi(\boldsymbol{r},t)$ which are everywhere defined, continuous, and infinitely differenciable C^∞. Also, we confine to wavefunctions that have a bounded domain (we can find the particle in a finite region of space).

We list the formal definition of a vector space which is used to define particular vector spaces.

Vector space

A **vector space** over a field F (set defined with addition and multiplication) is a non-empty set V together with a *vector addition* and a *scalar multiplication* that satisfies eight axioms. The elements of V are called vectors and the elements of F are caleld scalars.

$$\begin{array}{l|l}
\text{Commutativity of vector addition} & \boldsymbol{u}+\boldsymbol{v}=\boldsymbol{v}+\boldsymbol{u} \\
\text{Associativity of vector addition} & (\boldsymbol{u}+\boldsymbol{v})+\boldsymbol{w}=\boldsymbol{u}+(\boldsymbol{v}+\boldsymbol{w}) \\
\text{Identity element of vector addition} & \exists \boldsymbol{0},\boldsymbol{v}\in V: \quad \boldsymbol{v}+\boldsymbol{0}=\boldsymbol{v} \\
\text{Inverse element of vector addition} & \forall \boldsymbol{v}\in V,\ \exists -\boldsymbol{v}\in V: \quad \boldsymbol{v}+(-\boldsymbol{v})=\boldsymbol{0} \\
\text{Associativity of scalar multiplication} & \alpha(\beta\boldsymbol{v})=(\alpha\beta)\boldsymbol{v} \\
\text{Distributivity over vector addition} & \alpha(\boldsymbol{u}+\boldsymbol{v})=\alpha\boldsymbol{u}+\alpha\boldsymbol{v} \\
\text{Distributivity over scalar addition} & (\alpha+\beta)\boldsymbol{v}=\alpha\boldsymbol{v}+\beta\boldsymbol{v} \\
\text{Identity element of scalar multiplication} & \boldsymbol{1v}=\boldsymbol{v}
\end{array} \tag{1.2}$$

When the scalar field is the real numbers, the vector space is called a real vector space, when the scalar field is the complex numbers, then is called a complex vector space.

Vector space $\mathscr{F}$

The set of wavefunctions $\mathscr{F}\in L^2$ is composed of sufficiently regular functions of L^2.

1.1.1 Scalar product

With each pair of orderer elements of $\mathscr{F}$, $(\varphi(\boldsymbol{r}),\psi(\boldsymbol{r}))$, we associate a *complex number*:

$$(\varphi,\psi) = \int d^3r\ \varphi^*(\boldsymbol{r})\psi(\boldsymbol{r}) \in \mathbb{C}\,. \tag{1.3}$$

Its properties are listed below:

Adjoint	Linear in the second term	Antilinear in the first term
$(\varphi, \psi) = (\psi, \varphi)^*$	$(\varphi, \lambda_1\psi_1 + \lambda_2\psi_2) = \lambda_1(\varphi, \psi_1) + \lambda_2(\varphi, \psi_2)$	$(\lambda_1\varphi_1 + \lambda_2\varphi_2, \psi) = \lambda_1^*(\varphi_2, \psi) + \lambda_2^*(\varphi_2, \psi)$

If $(\varphi, \psi) = 0$, then $\varphi(\boldsymbol{r})$ and $\psi(\boldsymbol{r})$ are said to be **orthogonal**. In addition, the scalar product of a vector with itself return its *norm squared*:

$$\text{Parseval's theorem} \qquad (\varphi, \varphi) = \int d^3r \, |\psi(\boldsymbol{r})|^2 \geq 0 \in \mathbb{R}. \tag{1.4}$$

We also have the Schwarz inequality defined with the norms:

$$|(\psi_1, \psi_2)| \leq \sqrt{(\psi_1, \psi_1)}\sqrt{(\psi_2, \psi_2)}. \tag{1.5}$$

1.1.2 Linear operators

A linear operator A is a mathematical entity which associates with every function $\phi(\boldsymbol{r}) \in \mathscr{F}$ another function $\phi'(\boldsymbol{r})$ linearly:

$$\begin{aligned} &\phi'(\boldsymbol{r}) = A\phi(\boldsymbol{r}) \\ &A[\lambda_1\phi_1(\boldsymbol{r}) + \lambda_2\phi_2(\boldsymbol{r})] = \lambda_1 A\phi_1(\boldsymbol{r}) + \lambda_2 A\phi_2(\boldsymbol{r}) \end{aligned} \tag{1.6}$$

Let A, B be two linear operators, their product AB on a vector corresponds to the application of B first, and then A acts on the new vector $\varphi(\boldsymbol{r}) = B\psi(\boldsymbol{r})$:

$$(AB)\psi(\boldsymbol{r}) = A[B\psi(\boldsymbol{r})]. \tag{1.7}$$

In general, the order of application matter and a way to quantify it is through the **commutator**:

$$\boxed{[A, B] = AB - BA}\,. \tag{1.8}$$

1.1.3 Discrete orthonormal bases in $\mathscr{F}$: $\{u_i(\boldsymbol{r})\}$

Definition of discrete orthonormal bases

Let be a countable set of function $\{u_1(\boldsymbol{r})\} \in \mathscr{F}$.

- This set is orthonormal if only the inner profuct of the same function returns a non-zero value:

  $$\text{Orthonormalization relation} \qquad \boxed{(u_i, u_j) = \int d^3r \; u_i^*(\boldsymbol{r})u_j(\boldsymbol{r}) = \delta_{ij}}\,, \tag{1.9}$$

  where δ_{ij} is the kronecker function:

  $$\delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}. \tag{1.10}$$

- It constitutes a **basis** if every function $\psi(\boldsymbol{r}) \in \mathscr{F}$ can be expanded in only **one way** in $\{u_i(\boldsymbol{r})\}$ as a linear combination:

  $$\text{Expansion} \qquad \boxed{\psi(\boldsymbol{r}) = \sum_i c_i u_i(\boldsymbol{r})}\,, \tag{1.11}$$

whose elements of projection c_i are obtained computing the scalar product $(u_j, \psi(x))$:

$$(u_j, \psi) = \left(u_j, \sum_i c_i u_i(\boldsymbol{r})\right) = \sum_i c_i (u_j, u_i) = \sum_i c_i \delta_{ij} = c_j.$$

Thus,

$$\text{Coefficient expansion} \qquad \boxed{c_i = (u_i, \psi) = \int d^3r\ u_i^*(\boldsymbol{r})\psi(\boldsymbol{r})}\,. \tag{1.12}$$

Once projected in $\{u_i(\boldsymbol{r})\}$ it is equivalent to specify $\psi(\boldsymbol{r})$ or the set of c_i, which represent $\psi(\boldsymbol{r})$ in the $\{u_i(\boldsymbol{r})\}$ basis. The 3D generalization is given in A-22-A-24.

The scalar product of two wavefunctions can also be expressed in terms of the coefficients of projection. Let be $\varphi(\boldsymbol{r}), \psi(\boldsymbol{r})$,

$$(\varphi, \psi) = \left[\sum_i b_i u_i, \sum_j c_j u_j\right] = \sum_{i,j} b_i^* c_j (u_i, u_j) = \sum_{i,j} b_i^* c_j \delta_{ij}. \tag{1.13}$$

Therefore, the scalar product is:

$$\text{Scalar product} \qquad \boxed{(\varphi, \psi) = \sum_i b_i^* c_i} \tag{1.14}$$

Its generalization for 3D is given in A-28.

Closure relation

Equation (1.9) is called *orthonormalization relation* over the set $\{u_i(\boldsymbol{r})\}$. There is another condition called *Closure relation*, which express the fact that this set constitutes a basis.

If $\{u_i(\boldsymbol{r})\} \in \mathscr{F}$, the any function $\psi(\boldsymbol{r}) \in \mathscr{F}$ is decomposed using equation (1.11):

$$\psi(\boldsymbol{r}) = \sum_i c_i u_i(\boldsymbol{r}) = \sum_i (u_i, \psi) u_i(\boldsymbol{r}) = \sum_i \left[\int d^3r'\ u_i^*(\boldsymbol{r}')\psi(\boldsymbol{r}')\right] u_i(\boldsymbol{r}) = \int d^3r'\ \psi(\boldsymbol{r}') \left[\sum_i u_i(\boldsymbol{r}) u_i^*(\boldsymbol{r}')\right]$$

This integration with sum will be $\psi(\boldsymbol{r})$ only when $\boldsymbol{r} = \boldsymbol{r}'$, which is characteristic of a delta function centered at $\boldsymbol{r} = \boldsymbol{r}'$. Thus, the only way to achieve that is that the sum must be a delta function $\delta(\boldsymbol{r} - \boldsymbol{r}')$ and we have

$$\text{Closure relation} \qquad \boxed{\sum_i u_i(\boldsymbol{r}) u_i^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}')}\,. \tag{1.15}$$

If an orthonormal set $\{u_i(\boldsymbol{r})\}$ satisfies the closure relation then it constitutes a basis.

1.1.4 Bases not belonging to $\mathscr{F}$

The $\{u_i(\boldsymbol{r})\}$ bases are composed of square-integrable functions. It can also be convenient to introduce bases of functions **not belonging** to $\mathscr{F}$ or L_2, but in terms of which any wavefunction $\psi(\boldsymbol{r})$ can nevertheless be expanded. We will discuss two examples: 1D plane wave, and delta functions, after which we will study continuous bases.

Plane waves

Consider a plane wave $v_p(x)$ with wave vector $p/\hbar$

$$v_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}. \tag{1.16}$$

The integral of $|v_p(x)|^2 = \frac{1}{2\pi\hbar}$ over $x \in \mathbb{R}$ diverges, therefore $v_p(x) \notin \mathscr{F}_x$. We shall designate $\{v_o(x)\}$ the set of all plane waves, with the continuous index $p \in (-\infty, \infty)$. The Fourier-pair equations

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\ \bar{\psi}(p) e^{ipx/\hbar}, \quad \text{and} \quad \bar{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\ \psi(x) e^{-ipx/\hbar},$$

can be rewritten with the definition of the plane wave:

$$\psi(x) = \int_{-\infty}^{\infty} dp\ \bar{\psi}(p) v_p(x), \tag{1.17}$$

$$\bar{\psi}(p) = (v_p, \psi) = \int_{-\infty}^{\infty} dx\ v_p^*(x)\psi(x). \tag{1.18}$$

The two formulas can be compared to equations (1.11) and (1.12). In this case, every function $\psi(x) \in \mathscr{F}_x$ can be expanded in only one way as a continuous linear combination of planes waves, whose components are given by (1.18). The set of these components constitutes a function of p, $\bar{\psi}(p)$, the Fourier transform of $\psi(x)$.

> $\bar{\psi}(p)$ is analogous to c_i, both represent the components of the same function $\psi(x)$ in two different bases: $\{v_p(x)\}$ and $\{u_i(x)\}$.

If we calculate the square of the norm of $\psi(x)$ we will get:

$$\text{Parseval's theorem} \qquad (\psi, \psi) = \int_{-\infty}^{\infty} dp\ |\bar{\psi}(p)|^2. \tag{1.19}$$

We can also show that $v_p(x)$ satisfy the closure relation:

$$\begin{aligned} \psi(x) &= \int_{-\infty}^{\infty} dp\ \bar{\psi}(p) v_p(x) = \int_{-\infty}^{\infty} dp\ (v_p, \psi) v_p(x) = \int_{-\infty}^{\infty} dp\ \left[\int_{-\infty}^{\infty} dx'\ v_p^*(x')\psi(x')\right] v_p(x) \\ &= \int_{-\infty}^{\infty} dx'\ \psi(x') \left[\int_{-\infty}^{\infty} dp\ v_p(x) v_p^*(x')\right]. \end{aligned}$$

The term inside the brackets corresponds to

$$\text{Closure relation} \qquad \boxed{\int_{-\infty}^{\infty} dp\ v_p(x) v_p^*(x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dp}{\hbar} e^{i\frac{p}{\hbar}(x-x')} \stackrel{(a)}{=} \delta(x - x')}\,. \tag{1.20}$$

In (a) the following relation was used:

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dk\ e^{iku} = \delta(u).$$

Equation (1.20) is analogous to (1.15). In the same way, we can derive the orthonormalization relation using (a):

$$(v_p, v_{p'}) = \int_{-\infty}^{\infty} dx\ v_p^*(x) v_{p'}(x) = \frac{1}{2\pi} \int \frac{dx}{\hbar} e^{i\frac{x}{\hbar}(p'-p)} = \delta(p-p').$$

Therefore,

$$\text{Orthonormalization relation} \qquad \boxed{(v_p, v_{p'}) = \delta(p-p')}\,. \tag{1.21}$$

Now instead of a kronecker delta, we have a delta function. If $p = p'$, the scalar product **diverges**: we see again that $v_p(x) \notin \mathscr{F}_x$. It is also sait that $v_p(x)$ is "orthonormalized in the Dirac sense". The generalization to three dimension is given by

$$v_{\boldsymbol{p}}(\boldsymbol{r}) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i\cdot\boldsymbol{p}/\hbar}. \tag{1.22}$$

The functions of $\{v_p(\boldsymbol{r})\}$ basis now depend on the thre continuous indices p_x, p_y, p_z condensed in $\boldsymbol{p}$. In addition,

$$\text{Expansion} \qquad \psi(\boldsymbol{r}) = \int d^3p\ \bar{\psi}(\boldsymbol{p}) v_{\boldsymbol{p}}(\boldsymbol{r}) \tag{1.23}$$

$$\text{Coefficient expansion} \qquad \bar{\psi}(\boldsymbol{p}) = (v_{\boldsymbol{p}}, \psi) = \int d^3r\ v_{\boldsymbol{p}}^*(\boldsymbol{r}) \psi(\boldsymbol{r}) \tag{1.24}$$

$$\text{Scalar product} \qquad (\varphi, \psi) = \int d^3p\ \bar{\varphi}^*(\boldsymbol{p}) \bar{\psi}(\boldsymbol{p}) \tag{1.25}$$

$$\text{Closure relation} \qquad \int d^3p\ v_{\boldsymbol{p}}(\boldsymbol{r}) v_{\boldsymbol{p}}^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') \tag{1.26}$$

$$\text{Orthornormalization relation} \qquad (v_{\boldsymbol{p}}, v_{\boldsymbol{p}'}) = \delta(\boldsymbol{p}-\boldsymbol{p}') \tag{1.27}$$

The $v_p(\boldsymbol{r})$ can be considered to constitute a **continuous** basis.

Delta function

We can also consider a set of functions of $\boldsymbol{r}$, $\{\xi_{\boldsymbol{r}_o}(\boldsymbol{r})\}$, labeled by the continuous index $\boldsymbol{r}_0 = (x_0, y_0, z_0)$ and defined by

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) = \delta(\boldsymbol{r}-\boldsymbol{r}_0). \tag{1.28}$$

Obviously, $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ is not square-integrable: $\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) \notin \mathscr{F}$.

Then, we can have the following

$$\text{Expansion} \qquad \psi(\boldsymbol{r}) = \int d^3r_0\ \psi(\boldsymbol{r}_0) \xi_{\boldsymbol{r}_0}(\boldsymbol{r}), \quad \text{and} \tag{1.29}$$

$$\text{Coefficient expansion} \qquad \psi(\boldsymbol{r}_0) = (\xi_{\boldsymbol{r}_0}, \psi) = \int d^3r\ \xi_{\boldsymbol{r}_0}^*(\boldsymbol{r}) \psi(\boldsymbol{r}). \tag{1.30}$$

The equations are analogous to equations (1.11) and (1.12).

$\psi(\boldsymbol{r}_0)$ is the equivalent of c_i, which represent the components of the same function $\psi(\boldsymbol{r})$ in two different bases: $\{\xi_{\boldsymbol{r}_0}(\boldsymbol{r})\}$ and $\{u_i(\boldsymbol{r})\}$.

We also list, the other formulas:

$$\text{Scalar product} \qquad (\varphi, \psi) = \int d^3 r_0 \; \varphi^*(\boldsymbol{r}_0)\psi(\boldsymbol{r}_0) \tag{1.31}$$

$$\text{Closure relation} \qquad \int d^3 r_0 \; \xi_{\boldsymbol{r}_0}(\boldsymbol{r})\xi^*_{\boldsymbol{r}_0}(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{1.32}$$

$$\text{Orthonormalization relation} \qquad (\xi_{\boldsymbol{r}_0}, \xi_{\boldsymbol{r}'_0}) = \delta(\boldsymbol{r}_0 - \boldsymbol{r}'_0) \tag{1.33}$$

The $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ can be considered to constitute a **continuous** basis.

A physical state must **always** correspond to a qaure-integrable wavefunction. In no case $v_p(\boldsymbol{r})$ and $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ can represent the state of a particle. They are nothing more than intermediaries, useful for calculations.

Continuous orthonormal bases

We will denote a continuous orthonormal basis to a set of function of $\boldsymbol{r}$, $\{w_\alpha(\boldsymbol{r})\}$, labeled by a continuous index α, which satisfy the closure and orthonormalization relations:

$$\text{Orthonormalization relation} \qquad (w_\alpha, w_{\alpha'}) = \int d^3 r \; w^*_\alpha(\boldsymbol{r})w_{\alpha'}(\boldsymbol{r}) = \delta(\alpha - \alpha') \tag{1.34}$$

$$\text{Closure relation} \qquad \int d\alpha \; w_\alpha(\boldsymbol{r})w^*_\alpha(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{1.35}$$

When $\alpha = \alpha'$, $(w_\alpha, w_{\alpha'})$ **diverges**. Therefore, $\omega_\alpha(\boldsymbol{r}) \notin \mathscr{F}$. Recall that this is a generalized continuous basis, so it can represent the plane waves and delta functions by setting $\alpha = \boldsymbol{p}$ and $\alpha = \boldsymbol{r}_0$, respectively.

In the case of mixed (discrete and continuous) basis $\{u_i(\boldsymbol{r}), w_\alpha(\boldsymbol{r})\}$, the orthonormalization relations are

$$\text{Orthonormalization relation for mixed basis} \qquad \begin{array}{l} (u_i, u_j) = \delta_{ij} \\ (w_\alpha, w_{\alpha'}) = \delta(\alpha - \alpha') \\ (u_i, w_\alpha) = 0 \end{array} . \tag{1.36}$$

And the closure relation becomes:

$$\text{Closure relation for mixed basis} \qquad \sum_i u_i(\boldsymbol{r})u^*_i(\boldsymbol{r}') + \int d\alpha \; w_\alpha(\boldsymbol{r})w^*_\alpha(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{1.37}$$

We also list the expansion, coefficient of expansion and the scalar product for the continuous basis:

$$\text{Expansion} \qquad \psi(\boldsymbol{r}) = \int d\alpha \; c(\alpha)w_\alpha(\boldsymbol{r}) \tag{1.38}$$

$$\text{Coefficient expansion} \qquad c(\alpha) = (w_\alpha, \psi) = \int d^3 r' \; w^*_\alpha(\boldsymbol{r}')\psi(\boldsymbol{r}') \tag{1.39}$$

$$\text{Scalar product} \qquad (\varphi, \psi) = \int d\alpha \; b^*(\alpha)c(\alpha) \tag{1.40}$$

The squared norm of the wavefunction with itself is then

$$\text{Parseval's theorem} \qquad (\psi, \psi) = \int d\alpha \, |c(\alpha)|^2. \tag{1.41}$$

Finally, all the formulas can thus be generalized from discrete basis of index i and continuous basis with index α (which can consider the plane wave and delta functions) through the following change of variables:

$$\text{Transformation } \{u_i(\boldsymbol{r})\} \longleftrightarrow \{w_\alpha(\boldsymbol{r})\} \qquad \boxed{\begin{aligned} & i \longleftrightarrow \alpha \\ & \sum_i \longleftrightarrow \int d\alpha \\ & \delta_{ij} \longleftrightarrow \delta(\alpha - \alpha') \end{aligned}} \tag{1.42}$$

Table 1.1 Fundamental formulas for discrete and continuous basis.

Property	Discrete basis $\{u_i(\boldsymbol{r})\}$	Continuous basis $\{w_\alpha(\boldsymbol{r})\}$
Scalar product	$(\varphi, \psi) = \sum_i b_i^* c_i$	$(\varphi, \psi) = \int d\alpha \, b^*(\alpha) c(\alpha)$
Parseval	$(\psi, \psi) = \sum_i \|c_i\|^2$	$(\psi, \psi) = \int d\alpha \, \|c(\alpha)\|^2$
Orthonormalization relation	$(u_i, u_j) = \delta_{ij}$	$(w_\alpha, w_{\alpha'}) = \delta(\alpha - \alpha')$
Closure relation	$\sum_i u_i(\boldsymbol{r}) u_i^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}')$	$\int d\alpha \, w_\alpha(\boldsymbol{r}) w_\alpha^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}')$
Expansion	$\psi(\boldsymbol{r}) = \sum_i c_i u_i(\boldsymbol{r})$	$\psi(\boldsymbol{r}) = \int d\alpha \, c(\alpha) w_\alpha(\boldsymbol{r})$
Components	$c_i = (u_i, \psi)$	$c(\alpha) = (w_\alpha, \psi)$

1.2 Dirac notation

Each quantum state of a particle will be characterized by a **state vector**, belonging to an abstract space $\mathscr{E}_{\boldsymbol{r}}$, called the **state space** of the particle. The fact that the space $\mathscr{F}$ is a subspace of L^2 means that $E_{\boldsymbol{r}}$ is a subspace of a Hilbert space.

The introduction of these quantities permits a generalization of the formalism. In fact, there exist physical systems whose quantum description cannot be given by a wavefunction.

State vector

The quantum state of any physical system is characterized by a state vector, belonging to a space $\mathscr{E}$ which is the state space of the system. The state space is the set of all of the possible states in which the system can exist.

1.2.1 Ket and Bra vectors

Ket vectors

Any element or vector of space $\mathscr{E}$ is called a **key vector** or ket, and is represented by the symbol $|\cdot\rangle$. We shall define the space $\mathscr{E}_{\boldsymbol{r}}$ of the states of a particle by associating with every square-integrable function $|psi(\boldsymbol{r})$ a ket vector $|\psi\rangle$ of $\mathscr{E}_{\boldsymbol{r}}$:

$$\psi(\boldsymbol{r}) \in \mathscr{F} \Longrightarrow |\psi\rangle \in \mathscr{E}_{\boldsymbol{r}}. \tag{1.43}$$

Altough $\mathscr{F}$ and $\mathscr{E}_{\boldsymbol{r}}$ are **isomorphic**, we shal carefully distinguish between them. We see that the $\boldsymbol{r}$-dependence no longer appears in $|\psi\rangle$: only appears ψ as an object that is used to extract information.

Dual space and bra vectors

A **linear function** χ is a linear operation which associantes a complex number with every ket $|\psi\rangle$:

$$\begin{aligned} &|\psi\rangle \in \mathscr{E} \xrightarrow{\chi} \chi(|\psi\rangle) \in \mathbb{C} \\ &\chi(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1\chi(|\psi_1\rangle) + \lambda_2\chi(|\psi_2\rangle). \end{aligned} \tag{1.44}$$

> A linear functional is an operator that returns a complex number, while a linear operator returns another ket (vector).

The set of linear functionals defined on $|\psi\rangle \in \mathscr{E}$ constitutes a vector space, which is called **dual space** of $\mathscr{E}$ and which will be symbolized by $\mathscr{E}^*$.

Any element, or vector of the space $\mathscr{E}^*$ is called a **bra vector**, or bra and is denoted by $\langle\cdot|$.

The bra acts as a linear operator over the ket, which can be used to define the scalar product to return a complex number:

$$\text{Scalar product} \qquad \boxed{\langle\varphi|\psi\rangle = (|\varphi\rangle, |\psi\rangle)}\,. \tag{1.45}$$

We then have similar properties for the scalar product:

$$\begin{array}{lll} \text{Adjoint} & \text{Linear to the second vector} & \text{Antilinear to the first vector} \\ \langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^* & \langle\varphi|\lambda_1\psi_1 + \lambda_2\psi_2\rangle = \lambda_1\langle\varphi|\psi_1\rangle + \lambda_2\langle\varphi|\psi_2\rangle & \langle\lambda_1\varphi_1 + \lambda_2\varphi_2|\psi\rangle = \lambda_1^*\langle\varphi_1|\psi\rangle + \lambda_2^*\langle\varphi_2|\psi\rangle \end{array} \tag{1.46}$$

Relation bra-ket

There is an antilinear relation between a ket and its bra, so that we have the following multiplications by a scalar for the vectors

$$|\lambda\psi\rangle = \lambda|\psi\rangle \in \mathscr{E} \Longrightarrow \langle\lambda\psi| = \lambda^*\langle\psi| \in \mathscr{E}^*, \quad \lambda \in \mathbb{C}. \tag{1.47}$$

Although to every ket there corresponds a bra, it is possible to find bras that have no corresponding kets such as delta functions and plane waves spaces. This dissymetry of the correspondence bra-ket is related to the existence of continuous basis for $\mathscr{F}_x$. This happens when the norm of the functions blow up making them not belong to $\mathscr{F}_x$, so we cannot associate a ket of $\mathscr{E}_x$ with them. Nervertheless, their scalar pdouct with a function of $\mathscr{F}_x$ is defined, and this permits us to assicate with them a linear function of $\mathscr{E}_x$: the bra belonging to $\mathscr{E}_x^*$. However, we can define **generalized kets**, defined using functions that are not L^2, but whose scalar product with every function of $\mathscr{F}_x$ exists.

When working with plane waves and delta functions, we assume the following approximation:

$$|\xi_{x_0}\rangle \overset{\text{Refers to}}{\longrightarrow} |\xi_{x_0}^{(\epsilon)}\rangle, \quad \text{and} \quad |v_{p_0}\rangle \overset{\text{Refers to}}{\longrightarrow} |v_{p_0}^{(L)}\rangle, \tag{1.48}$$

where ϵ is very small and L very large compared to all other lengths of the problem, so we are always working in $\mathscr{E}_x$.

Note that

$$\begin{array}{l} \xi_{x_0}^{(\epsilon)}(x) \in \mathscr{F}_x \Longleftrightarrow |\xi_{x_0}^{(\epsilon)}\rangle \in \mathscr{E}_x \\ \lim\limits_{\epsilon\to 0} |\xi_{x_0}^{(\epsilon)}\rangle \notin \mathscr{E}_x \\ \lim\limits_{\epsilon\to 0} \langle\xi_{x_0}^{(\epsilon)}| = \langle\xi_{x_0}| \in \mathscr{E}_x^* \\ |\psi\rangle \in \mathscr{E}_x \Longrightarrow \langle\xi_{x_0}|\psi\rangle = \psi(x_0) \end{array}, \quad \text{and} \quad \begin{array}{l} v_{p_0}^{(L)}(x) \in \mathscr{F}_x \Longleftrightarrow |v_{p_0}^{(L)}\rangle \in \mathscr{E}_x \\ \lim\limits_{L\to\infty} |v_{p_0}^{(L)}\rangle \notin \mathscr{E}_x \\ \lim\limits_{L\to\infty} \langle v_{p_0}^{(L)}| = \langle v_{p_0}| \in \mathscr{E}_x^* \\ |\psi\rangle \in \mathscr{E}_x \Longrightarrow \langle v_{p_0}|\psi\rangle = \bar{\psi}(p_0) \end{array} \tag{1.49}$$

In general, the dual space $\mathscr{E}^*$ and the stae space $\mathscr{E}$ are not isomorphic, exept that $\mathscr{E}$ is finite-dimensional. Although to each ket there corresponds a bra, the converse is not true. In addition to use vector of $\mathscr{E}$ (whose norm is finite), **generalized kets** with infinite norms but whose scalar product with every ket of $\mathscr{E}$ is finite. Thus, to each bra of $\mathscr{E}^*$ there will correpsond a ket. But generalized kets do not represent physical states of the system.

1.2.2 Linear operators

A linear operator A associates with every ket $|\psi\rangle \in \mathscr{E}$ another ket $|\psi'\rangle \in \mathscr{E}$ linearly:

$$|\psi'\rangle = A|\psi\rangle \tag{1.50}$$

$$A(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1 A|\psi_1\rangle + \lambda_2 A|\psi_2\rangle. \tag{1.51}$$

The product of two linear operators AB is defined by first acting B in the ket $|\psi\rangle$, and then A:

$$(AB)|\psi\rangle = A(B|\psi\rangle). \tag{1.52}$$

The commutator express the degree of difference between the change of order of operation:

$$[A, B] = AB - BA\,. \tag{1.53}$$

We call the **matrix element** of A between $|\varphi\rangle$ and $|\psi\rangle$, the scalar product that measure the collinearity between the action of the operator onto $|\varphi\rangle$:

$$\langle\varphi|A|\psi\rangle \in \mathbb{C}\,. \tag{1.54}$$

Projector

Lets assume that $\langle\psi|\psi\rangle = 1$ (normalized), we define the **projector** as an operator that projects a ket into another ket:

$$P_\psi = |\psi\rangle\langle\psi| \tag{1.55}$$

When it acts into a vector, it first compute the scalar product and the assign the value to the vector from which the product was computed:

$$P_\psi|\varphi\rangle = |\psi\rangle \underbrace{\langle\psi|\varphi\rangle}_{\text{number}}.$$

It is also *idempotent*, which means that

$$P_\psi^2 = P_\psi P_\psi = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = P_\psi. \tag{1.56}$$

The most generalized form is project a ket into a orthonormalized ($\langle\varphi_i|\varphi_j\rangle = \delta_{ij}$) subespace $\{\varphi_q\} \in \mathscr{E}_q \subseteq \mathscr{E}$. Let P_q be then the linear operator

$$\boxed{P_q = \sum_{i=1}^{q} |\varphi_i\rangle\langle\varphi_i|}\,. \tag{1.57}$$

It then takes the ket, and compute the projection to every vector $|\varphi_i\rangle$ and the form a linear combination.

1.2.3 Hermitian conjugation (adjoint)

There is also possible to define actions of A on bras as $\langle\chi|A$, whose order is important.

We can also link with every linear operator A another linear operator $A^\dagger$, caled the adjoint operator (or Hermitian conjugate) of A. The operatoe A associates with it another ket $|\psi'\rangle = A|\psi\rangle \in \mathscr{E}$. The correspondende between kets and bras permits us to define the action of operator $A^\dagger$ on the bras:

$$|\psi\rangle \text{ corresponds to } \langle\psi| \Longrightarrow |\psi'\rangle = A|\psi\rangle \text{ corresponds to } \langle\psi'| = \langle\psi|A^\dagger. \tag{1.58}$$

The relation $\langle\psi'| = \langle\psi|A^\dagger$ is **linear**, as

$$A(\lambda_1^*|\psi_1\rangle + \lambda_2^*|\psi_2\rangle) = \lambda_1^* A|\psi_1'\rangle + \lambda_2^* A|\psi_2'\rangle \text{ corresponds to } (\lambda_1\langle\psi_1| + \lambda_2\langle\psi_2|)A^\dagger = \lambda_2\langle\psi_1|A^\dagger + \lambda_2\langle\psi_2|A^\dagger.$$

Therefore, $A^\dagger$ is a linear operator defined by

$$|\psi'\rangle = A|\psi\rangle \Longleftrightarrow \langle\psi'| = \langle\psi|A^\dagger, \tag{1.59}$$

which also implies that

$$\langle\psi|A^\dagger|\varphi\rangle = \langle\varphi|A|\psi\rangle^*. \tag{1.60}$$

Properties

$$\begin{aligned} &(A^\dagger)^\dagger = A \\ &(\lambda A)^\dagger = \lambda^* A^\dagger \\ &(A+B)^\dagger = A^\dagger + B^\dagger \\ &(AB)^\dagger = B^\dagger A^\dagger \end{aligned}$$

Hermitian conjugation in Dirac notation

A ket $|\psi\rangle$ and its corresponding bra $\langle\psi|$ are said to be Hermitian conjugates of each other. In the same manner, $A^\dagger$ is also called Hermitian conjugate operator of A.

The operation of Hermitian conjugate is followed by a very simple rule:

Rule of Hermitian conjugate

To obtain the adjoint of any expression composed f constantes, kets, bras, and operators, one must:

Replace	$\begin{cases} \text{the constants by their complex conjugates} \\ \text{the kets by the bras associated} \\ \text{the bras by the kets associated} \\ \text{the operators by their adjoints} \end{cases}$
Reverse the order of the factors	Only constants can move around (commute)

As an example,

$$\big(\lambda\langle u|A|v\rangle|w\rangle\langle\psi|\big)^\dagger = |\psi\rangle\langle w|\langle v|A^\dagger|u\rangle \quad \overbrace{\lambda^*}^{\text{can move around}}$$

Hermitian operators

An operator A is said to be Hermitian if $A = A^\dagger$, which stasify the following relations:

$$\langle\psi|A|\varphi\rangle = \langle\varphi|A|\psi\rangle^* \quad \text{and}| \quad \langle A\varphi|\psi\rangle = \langle\varphi|A\psi\rangle.$$

In addition, the projector P_ψ is an Hermitian operator:

$$P_\psi^* = |\psi\rangle\langle\psi| = P_\psi. \tag{1.61}$$

The product of two Hermitian operators A, B is Hermitian only if $[A, B] = 0$.

1.3 Representations in state space

Choosing a representation means choosing and orthonormal (discrete or continuous) basis in the state space $\mathscr{E}$. Vectors and operators are then represented in this basis by *numbers*: components for the vectors, matrix elements for the operators.

We now translate all properties such as orthonormaliation relation and closure relation to the Dirac notation.

1.3.1 Relations characteristic of an orthonormal basis

Orthonormalization relation

A set of kets, discrete $\{|u_i\rangle\}$ or continuous $\{|w_\alpha\rangle\}$ is said to be orthonotmal if they satisfy the following equation:

$$\text{Orthonormalization relation} \qquad \begin{array}{l} \langle u_i|u_j\rangle = \delta_{ij} \\ \langle w_\alpha|w_{\alpha'}\rangle = \delta(\alpha-\alpha') \end{array}. \tag{1.62}$$

As can be seen, for a continuous set $\langle w_\alpha|w_\alpha\rangle$ **does not exists**: the $|w_\alpha\rangle$ have an infinite norm and therefore not belong to $\mathscr{E}$. Nevertheless, the vectors of $\mathscr{E}$ can be expanded on the $|w_\alpha\rangle$. It is useful then to accept $|w_\alpha\rangle$ as *generalized kets*.

Closure relation

A discrete or continuous set constitutes a basis if every ket $|\psi\rangle \in \mathscr{E}$ has a **unique** expansion on $|u_i\rangle$ or $|w_\alpha\rangle$:

$$\text{Closure relation} \quad \boxed{\begin{aligned} |\psi\rangle &= \sum_i c_i |u_i\rangle \\ |\psi\rangle &= \int d\alpha\ c(\alpha)|w_\alpha\rangle \end{aligned}}, \tag{1.63}$$

whose components are obtained multiplying $\langle u_j|$ ($\langle \omega_{\alpha'}|$) in the closure relation and using equation (1.62):

$$\text{Coefficient expansion} \quad \boxed{\begin{aligned} \langle u_j|\psi\rangle &= c_j \\ \langle w_{\alpha'}|\psi\rangle &= c(\alpha') \end{aligned}}. \tag{1.64}$$

We can reexpress the expansion employing the coefficient expansion equations:

$$|\psi\rangle = \sum_i c_i|u_i\rangle = \sum_i \langle u_i|\psi\rangle|u_i\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle = \left[\sum_i |u_i\rangle\langle u_i|\right]|\psi\rangle = P_{\{u_i\}}|\psi\rangle,$$

$$|\psi\rangle = \int d\alpha\ c(\alpha)|w_\alpha\rangle = \int d\alpha\ \langle w_\alpha|\psi\rangle|w_\alpha\rangle = \int d\alpha\ |w_\alpha\rangle\langle w_\alpha|\psi\rangle = \left[\int d\alpha\ |w_\alpha\rangle\langle w_\alpha|\right]|\psi\rangle = P_{\{w_\alpha\}}|\psi\rangle.$$

We then have the projector onto a discrete and continuous basis:

$$\text{Projectors} \quad \boxed{\begin{aligned} P_{\{u_i\}} &= \sum_i |u_i\rangle\langle u_i| = \mathbb{1} \\ P_{\{w_\alpha\}} &= \int d\alpha\ |w_\alpha\rangle\langle w_\alpha| = \mathbb{1} \end{aligned}} \quad \text{Closure relation,} \tag{1.65}$$

where $\mathbb{1}$ denotes the identiy operator in $\mathscr{E}$. These relations express the fact that $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ constitute bases.

Table 1.2 Fundamental formulas for calculation in the $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ representations.

$\{\|u_i\rangle\}$ representation	$\{\|w_\alpha\rangle\}$ representation
$\langle u_i\|u_j\rangle = \delta_{ij}$	$\langle w_\alpha\|w_{\alpha'}\rangle = \delta(\alpha - \alpha')$
$P_{\{u_i\}} = \sum_i \|u_i\rangle\langle u_i\| = \mathbb{1}$	$P_{\{w_\alpha\}} = \int d\alpha\ \|w_\alpha\rangle\langle w_\alpha\| = \mathbb{1}$

1.3.2 Representation of kets and bras

In the $\{|u_i\rangle\}$ basis, the ket $|\psi\rangle$ is represented by a set of its components $x_i\langle u_i|psi\rangle$. These numbers are arranged vertically to form a column matrix. On the other hand, for continuous basis $\{|w_\alpha\rangle\}$, the ket $|\psi\rangle$ is represented by a continuous **infinity** of numbers $c(\alpha) = \langle w_\alpha|\psi\rangle$: a function of α. We then draw a vertical axis with the values of $c(\alpha)$:

$$|\psi\rangle_{\{|u_i\rangle\}} = \mathbb{1}|\psi\rangle = P_{\{|u_i\rangle\}}|\psi\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle = \sum_i c_i|u_i\rangle,$$

$$|\psi\rangle_{\{|w_\alpha\rangle\}} = \mathbb{1}|\psi\rangle = P_{\{|w_\alpha\rangle\}}|\psi\rangle = \int d\alpha\ |w_\alpha\rangle\langle w_\alpha|\psi\rangle = \int d\alpha\ c(\alpha)|\psi\rangle.$$

Then,

$$|\psi\rangle_{\{|u_i\rangle\}} = \begin{bmatrix} \langle u_1|\psi\rangle \\ \langle u_2|\psi\rangle \\ \vdots \\ \langle u_i|\psi\rangle \\ \vdots \end{bmatrix}, \quad \text{and} \quad |\psi\rangle_{\{|w_\alpha\rangle\}} = \begin{array}{c} \\ \\ \alpha\downarrow \\ \\ \\ \end{array} \begin{bmatrix} \vdots \\ \vdots \\ \langle w_\alpha|\psi\rangle \\ \vdots \\ \vdots \end{bmatrix}. \tag{1.66}$$

Something similar happens to the respective bras:

$$\langle\varphi|_{\{|u_i\rangle\}} = \langle\varphi|\mathbb{1} = \langle\varphi|P_{\{|u_i\rangle\}} = \sum_i \langle\varphi|u_i\rangle\langle u_i| = \sum_i b_i^* \langle u_i|,$$

$$\langle\varphi|_{\{|w_\alpha\rangle\}} = \langle\varphi|\mathbb{1} = \langle\varphi|P_{\{|w_\alpha\rangle\}} = \int d\alpha\ \langle\varphi|w_\alpha\rangle\langle w_\alpha| = \int d\alpha\ b^*(\alpha)\langle\varphi|.$$

We can see that the components of the bra are the complex conjugates of the components $b_i = \langle u_i|\varphi\rangle$ and $b(\alpha) = \langle w_\alpha|\varphi\rangle$ of the ket $|\varphi\rangle$ associated with $\langle\varphi|$.

Let us then arrange them horizontally, to form a row matrix:

$$\langle\varphi|_{\{|u_i\rangle\}} = \begin{bmatrix} \langle\varphi|u_1\rangle & \langle\varphi|u_2\rangle & \cdots & \langle\varphi|u_i\rangle & \cdots \end{bmatrix}, \quad \text{and} \tag{1.67}$$

$$\langle\varphi|_{\{|w_\alpha\rangle\}} = \begin{array}{ccccc} & & \alpha & & \\ & & \rightarrow & & \\ \end{array} \begin{bmatrix} \cdots & \cdots & \langle\varphi|w_\alpha\rangle & \cdots & \cdots \end{bmatrix}. \tag{1.68}$$

The scalar product is then given by a **matrix multiplication**:

$$\langle\varphi|\psi\rangle = \langle\varphi|\mathbb{1}|\psi\rangle = \langle\varphi|P_{\{u_i\}}|\psi\rangle = \sum_i \langle\varphi|u_i\rangle\langle u_i|\varphi\rangle = \sum_i b_i^* c_i \tag{1.69}$$

$$\langle\varphi|\psi\rangle = \langle\varphi|\mathbb{1}|\psi\rangle = \langle\varphi|P_{\{w_\alpha\}}|\psi\rangle = \int d\alpha\ \langle\varphi|w_\alpha\rangle\langle w_\alpha|\psi\rangle = \int d\alpha\ b^*(\alpha)c(\alpha). \tag{1.70}$$

1.3.3 Representation of operators

Representation of A by a square matrix

Given a linear operator A, we can in $\{|u_i\rangle\}$ or $\{|w_\alpha\rangle\}$ basis, associate with it a series of numbers defined by

$$A_{ij} = \langle u_i|A|u_j\rangle, \quad \text{or} \quad A(\alpha,\alpha') = \langle w_\alpha|A|w_{\alpha'}\rangle. \tag{1.71}$$

They are arranged into a square matrix, as

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1j} & \cdots \\ A_{21} & A_{22} & \cdots & A_{2j} & \cdots \\ \vdots & \vdots & & \vdots & \\ A_{i1} & A_{i2} & \cdots & A_{ij} & \cdots \\ \vdots & \vdots & & \vdots & \end{bmatrix}, \quad \text{or} \quad \begin{array}{cc} & \begin{array}{cccc} & & \alpha' & \\ & & \longrightarrow & \end{array} \\ \alpha\downarrow & \begin{bmatrix} & & \vdots & \\ & & \vdots & \\ \cdots & \cdots & A(\alpha,\alpha') & \cdots \\ & & \vdots & \end{bmatrix} \end{array}. \tag{1.72}$$

For the case of the matrix representing the operator AB in the $\{|u_i\rangle\}$ basis, we have:

$$\langle u_i|AB|u_j\rangle = \langle u_i|A\mathbb{1}B|u_j\rangle = \langle u_i|AP_{\{u_k\}}B|u_j\rangle = \sum_k \langle u_i|A|u_k\rangle\langle u_k|B|u_j\rangle = \sum_k A_{ik}B_{kj}.$$

Representation of the ket $|\psi'\rangle = A|\psi\rangle$

Knowing the componetns of $|\psi\rangle$ and the matrix elements of A in a given representation, how can we calculate the components of $|\psi'\rangle = S|\psi\rangle$ in the same representation?

We know that in the $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ basis, we have

$$c_i' = \langle u_i|\psi'\rangle = \langle u_i|A|\psi\rangle, \quad \text{and} \quad c'(\alpha) = \langle w_\alpha|\psi'\rangle.$$

Inserting the closure relation between A and $|\psi\rangle$:

$$c_i' = \langle u_1|A\mathbb{1}|\psi\rangle = \langle u_i|AP_{\{u_j\}}|\psi\rangle = \sum_j \langle u_i|A|u_j\rangle\langle u_j|\psi\rangle = \sum_j A_{ij}c_j$$
$$c'(\alpha) = \langle w_\alpha|A\mathbb{1}|\psi\rangle = \int d\alpha' \ \langle w_\alpha|A|w_{\alpha'}\rangle\langle w_{\alpha'}|\psi\rangle = \int d\alpha' \ A(\alpha,\alpha')c(\alpha').$$

We see that the column matrix representing $|\psi'\rangle$ is equal to the matrix multiplication of the column matrix $|\psi\rangle$ and the square matrix A.

Expression for the number $\langle\varphi|A|\psi\rangle$

On the other hand, we can derive an expression for $\langle\varphi|A|\psi\rangle$ for both basis:

$$\begin{aligned}\langle\varphi|A|\psi\rangle =& \langle\varphi|P_{\{u_i\}}AP_{\{u_j\}}|\psi\rangle = \sum_{i,j}\langle\varphi|u_i\rangle\langle u_i|A|u_j\rangle\langle u_j|\psi\rangle = \sum_{i,j} b_i^* A_{ij}c_j,\\ &\langle\varphi|P_{\{w_\alpha\}}AP_{\{w_{\alpha'}\}}|\psi\rangle = \iint d\alpha\, d\alpha' \ \langle\varphi|w_\alpha\rangle\langle w_\alpha|A|w_{\alpha'}\rangle\langle w_{\alpha'}|\psi\rangle = \iint d\alpha\, d\alpha' \ b^*(\alpha)A(\alpha,\alpha')c(\alpha').\end{aligned}$$

Thus, the term $\langle\varphi|A|\psi\rangle$ which is a number, can be computed as a matrix multiplication of the column vector $|\psi\rangle$ by the matrix A, and then by the row vector $\langle\varphi|$.

Matrix representation of $A^\dagger$

The adjoint of A can also be written as:

$$\begin{aligned}(A^\dagger)_{ij} &= \langle u_i|A^\dagger|u_j\rangle = \langle u_j|A|u_i\rangle^* = A_{ji}^*\\ A^\dagger(\alpha,\alpha') &= \langle w_\alpha|A^\dagger|w_{\alpha'}\rangle = \langle w_{\alpha'}|A|w_\alpha\rangle^* = A^*(\alpha',\alpha).\end{aligned} \tag{1.73}$$

The matrices representing A and $A^\dagger$ are then Hermitian conjugates of each other.

If A is Hermitian, then $A_{ij} = A_{ji}^*$ and $A(\alpha,\alpha') = A^*(\alpha',\alpha)$. A hermitian operator is therefore represented by a Hermitian matrix. For $i = j$, $\alpha = \alpha'$ we see that $A_{ii} = A_{ii}^*$, $A(\alpha,\alpha) = A^*(\alpha,\alpha)$. Thus,

The diagonal elements of a Hermitian matrix are therefore always real numbers.

1.3.4 Change of representation

We can representate a ket $|\psi\rangle$ in different bases, similar to representing a point in space by cartesian and spherical coordinates. The relation of these two representation allow us to turn from one to the other easily.

If we assume an old discrete basis $\{|u_i\rangle\}$ to a new one $\{|t_k\rangle\}$, the change of basis is defined by specifying the components $S_{ik} = \langle u_i|t_k\rangle$ of each kets of the new basis in terms of the kets of the old one. The adjoint is: $(S^\dagger)_{ki} = (S_{ik})^* = \langle t_k|u_i\rangle$. This transformation matrix is **unitary**: $S^\dagger S = SS^\dagger = I$.

We will derive the transformation for a ket, a bra, and the matrix elements of an operator using the closure relation of each basis as explained in the derivation.

$$\begin{aligned}
\langle t_k|\psi\rangle &= \langle t_k|\mathbb{1}|\psi\rangle = \langle t_k|P_{\{u_i\}}|\psi\rangle = \sum_i \langle t_k|u_i\rangle\langle u_i|\psi\rangle = \sum_i S^\dagger_{ki}\langle u_i|\psi\rangle \\
\langle u_i|\psi\rangle &= \langle u_i|\mathbb{1}|\psi\rangle = \langle u_i|P_{\{t_k\}}|\psi\rangle = \sum_k \langle u_i|t_k\rangle\langle t_k|\psi\rangle = \sum_i S_{ik}\langle t_k|\psi\rangle \\
\langle \psi|t_k\rangle &= \langle \psi|\mathbb{1}|t_k\rangle = \langle \psi|P_{\{u_i\}}|t_k\rangle = \sum_i \langle \psi|u_i\rangle\langle u_i|t_k\rangle = \sum_i \langle \psi|u_i\rangle S_{ik} \\
\langle \psi|u_i\rangle &= \langle \psi|\mathbb{1}|u_i\rangle = \langle \psi|P_{\{t_k\}}|u_i\rangle = \sum_k \langle \psi|t_k\rangle\langle t_k|u_i\rangle = \sum_k \langle \psi|t_k\rangle S^\dagger_{ki} \\
A_{kl} &= \langle t_k|A|t_l\rangle = \langle t_k|\mathbb{1}A\mathbb{1}|t_l\rangle = \langle t_k|P_{\{u_i\}}AP_{\{u_j\}}|t_l\rangle = \sum_{i,j} \langle t_k|u_i\rangle\langle u_i|A|u_j\rangle\langle u_j|t_l\rangle = \sum_{i,j} S^\dagger_{ki}A_{ij}S_{jl} \\
A_{ij} &= \langle u_i|A|u_j\rangle = \langle u_i|\mathbb{1}A\mathbb{1}|u_j\rangle = \langle u_i|P_{\{t_k\}}AP_{\{t_l\}}|u_j\rangle = \sum_{k,l} \langle u_i|t_k\rangle\langle t_k|A|t_l\rangle\langle t_l|u_j\rangle = \sum_{k,l} S_{ik}A_{kl}S^\dagger_{lj}.
\end{aligned}$$

The final results are shown in table

Table 1.3 Transformation of a ket, bra, and matrix elements from one basis to another.

Transformation	Expression
Ket components $\{u_i\} \longrightarrow \{t_k\}$ representation	$\langle t_k\|\psi\rangle = \sum_i S^\dagger_{ki}\langle u_i\|\psi\rangle$
Ket components $\{t_k\} \longrightarrow \{u_i\}$ representation	$\langle u_i\|\psi\rangle = \sum_i S_{ik}\langle t_k\|\psi\rangle$
Bra components $\{u_i\} \longrightarrow \{t_k\}$ representation	$\langle \psi\|t_k\rangle = \sum_i \langle \psi\|u_i\rangle S_{ik}$
Bra components $\{t_k\} \longrightarrow \{u_i\}$ representation	$\langle \psi\|u_i\rangle = \sum_k \langle \psi\|t_k\rangle S^\dagger_{ki}$
Matrix elements $\{u_{i,j}\} \longrightarrow \{t_{k,l}\}$ representation	$A_{kl} = \sum_{i,j} S^\dagger_{ki}A_{ij}S_{jl}$
Matrix elements $\{t_{k,l}\} \longrightarrow \{u_{i,j}\}$ representation	$A_{ij} = \sum_{k,l} S_{ik}A_{kl}S^\dagger_{lj}$

1.4 Eigenvalue equations. Observables

1.4.1 Eigenket and eigenbra equations

$|\psi\rangle$ is said to be an **eigenvector** (or eigenket) of the linear operator A if

$$\text{Eigenket equation of } A \qquad \boxed{A|\psi\rangle = \lambda|\psi\rangle, \quad \lambda \in \mathbb{C}}\,. \tag{1.74}$$

This eigenketequation possesses solutions only when λ takes on certain values, called **eigenvalues** of A. The set of the eigenvalues is called **spectrum** of A.

Collinear of an eigenvector is also an eigenvector

If $|\psi\rangle$ is an eigenvector of A with eigenvalue λ, then $\alpha|\psi\rangle,\ \alpha \in \mathbb{C}$ is also an eigenvector of A.

The eigenvalue λ is called *non-degenerate* (or simple) when its corresponding eigenvector is **unique** to within a constant factor (collinear). On the other hand, if there exists at least two linearly independent eigenkets with the **same** eigenvalue, the eigenvalue is said to be *degenerate*. Its *degree of degeneracy* g is then the number of linearly independent eigenvectors $|\psi^i\rangle,\ i = \{1, 2, \cdots, g\}$ associated with it.

The set of eigenkets associated with a degenerate eigenvalue constitutes a *g-dimensional vector space* called **eigensubspace** of λ.

Taking the adjoint of the eigeketnequation yields its corresponding form to eigenbraequation

$$\text{Eigenbra equation of } A^\dagger \qquad \boxed{\langle\psi|A^\dagger = \lambda^*\langle\psi|}\,. \tag{1.75}$$

If $|\psi\rangle$ is an eigenket of A with λ, it can also be said that $\langle\psi|$ is an eigenbra of $A^\dagger$ with λ^*.

Finding the eigenvalues and eigenvector in an operator

Assuming the state space is of finite dimension N, granting the generalization to an infinite-dimensional state space.

Choosing $\{|u_i\rangle\}$, lets us project the vector (1.74) onto the various orthonormal basis vectors $|u_i\rangle$:

$$\langle u_i|A|\psi\rangle = \lambda\langle u_i|\psi\rangle. \tag{1.76}$$

Inserting the closure relation between A and $|\psi\rangle$:

$$\langle u_i|A\mathbb{1}|\psi\rangle = \sum_j \underbrace{\langle u_i|A|u_j\rangle}_{A_{ij}}\underbrace{\langle u_j|\psi\rangle}_{c_j} = \lambda\underbrace{\langle u_i|\psi\rangle}_{c_i} \longrightarrow \boxed{\sum_j [A_{ij} - \lambda\delta_{ij}]c_j = 0}\,. \tag{1.77}$$

Equation (1.77) is a system of equations with N equations and N unknowns c_j. It has non-trivial solution iff its characteristic equation is zero:

$$\text{Characteristic equation of the eigenket equation} \qquad \boxed{P(\lambda) = \det[A - \lambda I] = 0}\,. \tag{1.78}$$

This expression enable us to determine the spectrum of A. The characteristic equation is **independent** of the representation chosen. Then, The eigenvalues of an operator are the roots λ of its Nth order characteristic equation $P(\lambda)$.

Determination of eigenvectors

Given a transformation $T(v) = Mv : \ V \in \mathbb{C}^{\mathbb{N}} \longrightarrow W \in \mathbb{C}^N$, the theorem says:

$$\dim(V) = \text{rank}(T) + \text{null}(T), \tag{1.79}$$

where

$$\begin{aligned} \dim(V) &= \text{Number of columns of V} \\ \text{rank}(T) &= \text{Number of independent equations (non zero rows)} \\ \text{null}(T) = \dim[\ker(T)] &= \text{Number of free variables, degree of freedom (dof)}. \end{aligned}$$

In our case, $T(v) = Mv = (A - \lambda I)v$ and $\dim(V) = N$.

Based on the nature of the eigenvalue, we can have different eigenvalues but also repeated. Therefore, we define the following useful quantities:

- **Algebraic multiplicity (AM)** Number of repetition of the eigenvalue (degree of degeneracy g).
- **Geometric multiplicity (GM)** Dimension of the subspace that the eigenvalues generate (how many linearly independent eigenvectors exist for that eigenvalue).

We then can have the following three cases:

- $AM = GM = 1$ Only one eigenvector corresponds to the eigenvalue (within a constant factor). At the moment of substituting an eigenvalue λ_0 into equation (1.77) there will be $\text{rank}(M) = N - 1$ independent equations so one equation is redundant. When this happens, $\text{null}(M) = 1$ free variable (or degree of freedom, dof) c_1 is available which can be defined arbitrarily and from which all other variables can be expressed.

  If we fix c_1, then all c_j are proportional to it:

  $$c_j = \alpha_j^0 c_1 \quad (\alpha_1^0 = 1). \tag{1.80}$$

  the $N-1$ coefficients $\alpha_j^0, \ j \neq 1$ are determined from the matrix elements A_{ij} and λ_0. The eigenvectors associated with λ_0 differ only by the value chosen for c_1. They are therefore all given by

  $$|\psi_0(c_1)\rangle = \sum_j \alpha_j^0 c_1 |u_j\rangle = c_1|\psi_0\rangle, \quad \text{with} \quad |\psi_0\rangle = \sum_j \alpha_j^0 |u_j\rangle. \tag{1.81}$$

  When λ_0 is simple, only one eigenvector corresponds to it.

Ejemplo 1.1 **Simple eigenvalues**

In the matrix

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$

the eigenvalues are $\lambda \in \{1, 2, 3\}$. Lets make $\lambda_0 = 1$ and replace it into the eigenvalue problem:

$$(A - \lambda I)v = (A - I)v = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{bmatrix} = 0$$

We see that there is no value in the first column, meaning that x_1 is free whereas $x_2 = x_3 = 0$. Therefore, the eigenvector is $v_1 = (1\ 0\ 0)$.

- $AM = GM > 1$ When evaluating λ_0, the system will have rank$(M) = N - p$ independent equations $(1 < p < q)$. To the eigenvalue λ_0 there corresponds an eigensubspace of dimension null$(M) = p$, and λ_0 is a p-fold degenerate eiganvalue.

  Assuming that for $\lambda = \lambda_0$ is composed of $N - 2$ linearly independent equations. These equations enable us to calculate the coefficients c_j in terms of any of them, for example c_1 and c_2:

  $$c_j = \beta_j^0 c_1 + \gamma_j^0 c_2.$$

  Al the eigenvectors associated with λ_0 are then of the form

  $$|\psi_0(c_1, c_2)\rangle = c_1|\psi_0^1\rangle + c_2|\psi_0^2\rangle, \quad \text{with} \quad |\psi_0^1\rangle = \sum_j \beta_j^0 |u_j\rangle, \quad |\psi_0^2\rangle = \sum_j \gamma_j^0 |u_j\rangle. \tag{1.82}$$

  The vectors $|\psi_0(c_1, c_2)\rangle$ do indeed constitute a two-dimensional vector space, this beeing characteristic of a two-fold degenerate eigenvalue.

- $AM > GM > 1$ In this case, the subspace is less than the degree of degeneracy and therefore not all degenerate eigenvectors are linearly independent. This means that there is not enough information to create a basis. However, techniques such as Jordan canonical form helps to create generalized eigenvector and to span the whole space.

When an operator is Hermitian, it can be shown that the degree of degeneracy p of an eigenvalue λ is always equal to the muliplicity of the corresponding root in the characteristic equations. In a space of finite dimension N, a Hermitian operator always has N linearly independent eigenvectors: this operator can therefore be diagonalized.

1.4.2 Observables

Properties of the eigenvalues and eigenvectors of a Hermitian operator

i) The eigenvalues of a Hermitian operator are real.

ii) Two eigenvectors of a Hermitian operator corresponding to two different eigenvalues are orthogonal.

Definition of a observable

Consider a Hermitian operator A with discrete spectrum. The degree of degeneracy of the eigenvalue a_n is denoted by g_n. We shall denote by $|\psi_n^i\rangle$ g_n linearly independent vectors chosen in the eigensubspace $\mathscr{E}_n$ of a_n:

$$A|\psi_n^i\rangle = a_n|\psi_n^i\rangle, \quad i = 1, 2, \cdots, g_n. \tag{1.83}$$

Every vector of $\mathscr{E}_n$ is orthogonal to every vector of another subspace $\mathscr{E}_{n'}$: $\langle\psi_n^i|\psi_{n'}^j\rangle = 0, \quad n \neq n'$.

Inside the subspace $\mathscr{E}_n$, the $|\psi_n^i\rangle$ can always be chosen orthonormal, such that

$$\langle\psi_n^i|\psi_n^j\rangle = \delta_{ij}. \tag{1.84}$$

If such a choise is made, the result is an orthonormal system of eigenvectors of A: the $|\psi_n^i\rangle$ satisfying the relations:

$$\langle\psi_n^i|\psi_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'}. \tag{1.85}$$

Observable

The Hermitian operator A is an **observable** if its eigenvectors **form a basis** in the state space:

Closure relation of an observable $$\sum_{n=1}^{\infty}\sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i| = \mathbb{1}\,. \tag{1.86}$$

The projector onto the subspace $\mathscr{E}_n$ is written as:

$$P_n = \sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i|. \tag{1.87}$$

The observable A is the ngiven by:

$$A = \sum_n a_n P_n\,. \tag{1.88}$$

Equation (1.86) can be generalized to include cases of continuous spectrum using the previous table of the first section.

If A has a mixed spectrum, then it is an observable if this system form a basis, that is, if

$$\sum_n \sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i| + \int_{\nu_1}^{\nu_2} d\nu\ |\psi_\nu\rangle\langle\psi_\nu| = \mathbb{1}. \tag{1.89}$$

The projector P_ψ is an observable

The projector $P_\psi = |\psi\rangle\langle\psi|$ is an observable. We know that it is Hermitian, and that its eigenvalues are 1 and 0, the first one is simple and the other infinitely degenerate. It can be shown that any ket $|\psi\rangle$ can be expanded on these eigenkets, therefore P_ψ is an observable.

1.4.3 Sets of commuting observables

Important theorems

Theorem I

If two operators A and B commute, and if $|\psi\rangle$ is an eigenvector of A, $B|\psi\rangle$ is aso an eigenvectr of A, with the same eigenvalue.

Another form:

If two operators A and B comute, every eigensubspace of A is globaly invariant under the action of B ($B|\psi\rangle$ belongs to the eigensubspace $\mathscr{E}_a$ of A, corresponding to the eigenvalue a).

Theorem II (consequence of theorem I)

If two observables A and B commute, and if $|\psi_1\rangle$ and $|\psi_2\rangle$ are two eigenvectors of A with different eigenvalues, the matrix element $\langle\psi_1|B|\psi_2\rangle$ is zero.

Theorem III

If two observables A and B commute, one can construct an orthonormal basis of the state spce with eigenvectors common to A and B.

Lets prove the theorem III. Consider two commuting observables A and B, with discrete spectrum. Since A is observable, there exists at least one orthonormal system of eigenvectors $|u_n^i\rangle$ which forms a basis in the state space:

$$A|u_n^i\rangle = a_n|u_n^i\rangle, \qquad \begin{array}{l} n = 1, 2, \cdots \\ i = 1, 2, \cdots, g_n \end{array} \tag{1.90}$$

We also have $\langle u_n^i|u_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'}$. What does the matrix look like which represent B in the $\{|u_n^i\rangle\}$ basis? We know that the matrix elements $\langle u_n^i|B|u_{n'}^{i'}\rangle$ are zero when $n \neq n'$ (theorem II). Let us arrange the basis vectors $|u_n^i\rangle$ in the order:

$$|u_1^1\rangle, |u_1^2\rangle, \cdots, |u_1^{g_1}\rangle;\ |u_2^1\rangle, \cdots, |u_2^{g_2}\rangle;\ |u_3^1\rangle, \cdots$$

Whe then obtain for B a block-diagonal matrix of the form:

$$\begin{array}{c|c|c|c|c} & \mathscr{E}_1 & \mathscr{E}_2 & \mathscr{E}_3 & \cdots \\ \hline \mathscr{E}_1 & \begin{matrix}\ddots & \ddots \\ \ddots & \ddots\end{matrix} & 0 & 0 & 0 \\ \hline \mathscr{E}_2 & 0 & \begin{matrix}\ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots\end{matrix} & 0 & 0 \\ \hline \mathscr{E}_3 & 0 & 0 & \ddots & 0 \\ \hline \vdots & 0 & 0 & 0 & \begin{matrix}\ddots & \ddots \\ \ddots & \ddots\end{matrix} \end{array} \tag{1.91}$$

Then the degeneracy of the eigenvalue is 1, then the block reduces to a 1×1 matrix. In the column associated with $|u_n\rangle$ all the other matrix elements are zero, this expresses the fact that $|u_n\rangle$ is an eigenvector common to A and B. When a_n is a g_n-degenerate eigenvalue of A, the block which represents B in $\mathscr{E}_n$ is not, in general, diagonal: the $|u_n^i\rangle$ are not, in general, eigenvector of B. The action of A in the g_n eigenvectors $|u_n^i\rangle$ reduces to $a_n|u_n^i\rangle$, the matrix representing the restriction of A wo within $\mathscr{E}_n$ is equal to $a_n I_{g_n \times g_n}$. The matrix representing the operator A in $\mathscr{E}_n$ is always diagonal and equal to $a_n I_{g_n \times g_n}$.

We use this property to obtain a basis of $\mathscr{E}_n$ composed of vectors that are also eigenvectors of B. The matrix representing B in $\mathscr{E}_n$ when the basis is chosen is

$$\{|u_n^i\rangle\ , \quad i = 1, 2, \cdots, g_n\}, \tag{1.92}$$

has for its elements:

$$\beta_{ij}^{(n)} = \langle u_n^i|B|u_n^j\rangle. \tag{1.93}$$

Thi matri is Hermitian, since B is a Hermitian operator. It is therefore diagonizable: one can find a new basis $\{|v_n^i\rangle;\ i = 1, 2, \cdots, g_n\}$ in which B is represented by a diagonal matrix:

$$\langle v_n^i|B|v_n^j\rangle = \beta_i^n \delta_{ij}. \tag{1.94}$$

This means that the new basis vectors in $\mathscr{E}_n$ are eigenvectors of B:

$$B|v_n^i\rangle = \beta i^{(n)}|v_n^i\rangle. \tag{1.95}$$

These vectors are automatically eigenvectors of A with an eigenvalue a_n since they belong to $\mathscr{E}_n$.

Eigenvectors of A associated with degenerate eigenvalues are not necessarily eigenvectors of B. It is always possible to choose, in every eigensubspace of A, a basis of eigenvectors common to A and B.

If we perform this operation in all the subsespaces $\mathscr{E}_n$, we obtain a bsis of $\mathscr{E}$, formed by eigenvectors common to A and B.

We shall denote by $|u_{n,p}^i\rangle$ the eigenvectors common to A an B:

$$A|u_{n,p}^i\rangle = a_n|u_{n,p}^i\rangle, \quad \text{and} \quad B|u_{n,p}^i\rangle = b_p|u_{n,p}^i\rangle. \tag{1.96}$$

The index i will be used to distinguish between different basis vectors which correspond to the same eigenvalues a_n and b_p.

Complete sets of commting observables (C.S.C.O.)

Consider an observable A and a basis $\mathscr{E}$ composed of eigenvectors $|u_n^i\rangle$ of A.

If none of the eigenvalues of A is degenerate, the various basis vectors of $\mathscr{E}$ can be labelled by the eigenvalue a_n (index i is not necessary). Thefroe, specifying the eigenvalue determines in a unique way the corresponding eigenvector. In other words, there exists only one basis of $\mathscr{E}$ formed by the eigenvectors of A. It is said that the observable A constitutes, by itself, a C.S.C.O.

On the other hand, if at least one eigenvalue of A is degenerate, specifying a_n is no longer always sufficient to characterize a basis vector: the basis of eigenvectors of A is not unique. One can choose any basis inside each of the degenerate eigensubspaces $\mathscr{E}_n$. We can choose another observable B which commute with A to construct an orthonormal basis of eigenvectors common to A and B. A and B form a C.S.C.O. if this basis is unique, that is, if to each of the possible pairs ofeigevalues $\{a_n, b_p\}$ there corresponds only one basis vector. For A and B to constitute a C.S.C.O., it is necessary and sufficient that, inside each of tese subspaces, all the g_n eigenvalues of B be distinct. We can add indifinitely observables until we reach the C.S.C.O.

A set of observables $A, B, C, \cdots$ is called a complete set of commuting observables if:

(i) all the observables commute by pairs.

(ii) specifying the eigenvalue of all the operators determines a unique common eigenvector. The ket then is denoted as $|a_n, b_p, c_r, \cdots\rangle$.

This means that they are C.S.C.O. if there exists a unique orthonormal basis of common eigenvectors.

Idenfitication of CSCOs is necessary in order to construct physically meaningful bases for $\mathscr{E}$. Knowing the CSCOs that are available tells the experimenter the possible sets of measurements that can be made to achieve this goal.

We list some CSCOs for specific problems. (table 31 anerson)

1.5 Two important examples of representation and observables

1.5.1 The $\{r\}$ and $\{p\}$ representations

Recall the following bases of $\mathscr{F}$. They are not composed of functions belonging to $\mathscr{F}$:

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) = \delta(\boldsymbol{r} - \boldsymbol{r}_0) \quad \text{and} \quad v_{\boldsymbol{p}_0}(\boldsymbol{r}) = (2\pi\hbar)^{-3/2} e^{\frac{i}{\hbar}\boldsymbol{p}_0 \cdot \boldsymbol{r}} \tag{1.97}$$

Every sufficiently regular equare-integrable function can be expanded in one or the other of these bases. The ket associted with $\xi_{\boldsymbol{r}_0}(\boldsymbol{r})$ and $v_{\boldsymbol{p}_0}(\boldsymbol{r})$ will be denoted as:

$$\xi_{\boldsymbol{r}_0}(\boldsymbol{r}) \Longleftrightarrow |\boldsymbol{r}_0\rangle \quad \text{and} \quad v_{\boldsymbol{p}_0}(\boldsymbol{r}) \Longleftrightarrow |\boldsymbol{p}_0\rangle. \tag{1.98}$$

Using these bases $\{\xi_{\boldsymbol{r}_0}(\boldsymbol{r})\}$ and $\{v_{\boldsymbol{p}_0}(\boldsymbol{r})\}$ of $\mathscr{F}$ we thus define in $\mathscr{E}_{\boldsymbol{r}}$ two representation: the $\{|\boldsymbol{r}_0\rangle\}$ and the $\{|\boldsymbol{p}_0\rangle\}$ representations.

Orthonormalization and closure relations

If we calculate the scalar product of two kets, we have

$$\langle \boldsymbol{r}_0|\boldsymbol{r}_0'\rangle = \int d^3r\ \xi^*_{\boldsymbol{r}_0}(\boldsymbol{r})\xi_{\boldsymbol{r}_0'}(\boldsymbol{r}) = \delta(\boldsymbol{r}_0 - \boldsymbol{r}_0') \quad \text{and} \quad \langle \boldsymbol{p}_0|\boldsymbol{p}_0'\rangle = \int d^3r\ v^*_{\boldsymbol{p}_0}(\boldsymbol{r})v_{\boldsymbol{p}_0'}(\boldsymbol{r}) = \delta(\boldsymbol{p}_0 - \boldsymbol{p}_0').$$

Thus, te baseses are therefore orthonormal in the extended sense. The fact that the set of the $|\boldsymbol{r}_0\rangle$ or that of $|\boldsymbol{p}_0\rangle$ constitutes a basis in $\mathscr{E}_{\boldsymbol{r}}$ can be expressed by a closure relation in $\mathscr{E}_{\boldsymbol{r}}$:

Orthonormality relation	Closure relation	
		(1.99)
$\langle \boldsymbol{r}_0|\boldsymbol{r}_0'\rangle = \delta(\boldsymbol{r}_0 - \boldsymbol{r}_0')$ $\langle \boldsymbol{p}_0, \boldsymbol{p}_0'\rangle = \delta(\boldsymbol{p}_0 - \boldsymbol{p}_0')$	$\int d^3r_0\ |\boldsymbol{r}_0\rangle\langle\boldsymbol{r}_0| = \mathbb{1}$ $\int d^3p_0\ |\boldsymbol{p}_0\rangle\langle\boldsymbol{p}_0| = \mathbb{1}$	(1.100)

Components of a ket

Consider a ket $|\psi\rangle$ corresponding to $\psi(\boldsymbol{r})$. We can expand it in each representation using the closure relation:

$$|\psi\rangle = \int d^3r_0\ |\boldsymbol{r}_0\rangle\langle\boldsymbol{r}_0|\psi\rangle, \quad \text{where} \quad \langle\boldsymbol{r}_0|\psi\rangle = \psi(\boldsymbol{r}_0) = \int d^3r\ \xi^*_{\boldsymbol{r}_0}(\boldsymbol{r})\psi(\boldsymbol{r}). \tag{1.101}$$

$$|\psi\rangle = \int d^3p_0\ |\boldsymbol{p}_0\rangle\langle\boldsymbol{p}_0|\psi\rangle, \quad \text{where} \quad \langle\boldsymbol{p}_0|\psi\rangle = \tilde{\psi}(\boldsymbol{p}_0) = \int d^3r\ v^*_{\boldsymbol{p}_0}(\boldsymbol{r})\psi(\boldsymbol{r}). \tag{1.102}$$

We see that $\tilde{\psi}(\boldsymbol{p}_0)$ is the Fourier transform of $\psi(\boldsymbol{r}_0)$. Each value corresponds to the components of $|\psi\rangle$ on the basis vector of the respective representation.

Now, we redefine the above bases to just $|\boldsymbol{r}\rangle$ and $|\boldsymbol{p}\rangle$:

$$\begin{array}{ll} \langle\boldsymbol{r}|\psi\rangle = \psi(\boldsymbol{r}) & \langle\boldsymbol{p}|\psi\rangle = \tilde{\psi}(\boldsymbol{p}) \\ \langle\boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}') & \langle\boldsymbol{p},\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}') \\ \displaystyle\int d^3r|\boldsymbol{r}\rangle\langle\boldsymbol{r}| = \mathbb{1} & \displaystyle\int d^3p\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \mathbb{1} \end{array} \tag{1.103}$$

Changing from $\{|\boldsymbol{r}\rangle\}$ to $\{|\boldsymbol{p}\rangle\}$ representation

Changing from one basis to the other brinds in the numbers:

$$\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \langle\boldsymbol{p}|\boldsymbol{r}\rangle^* = \int d^3r'\ \langle\boldsymbol{r}|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\boldsymbol{p}\rangle = \int d^3r'\ \delta(\boldsymbol{r}-\boldsymbol{r}')(2\pi\hbar)^{-3/2}e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}'} = (2\pi\hbar)^{-3/2}e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}. \tag{1.104}$$

A given ket $|\psi\rangle$ is represented by $\langle\boldsymbol{r}|\psi\rangle = \psi(\boldsymbol{r})$ in the $\{|\boldsymbol{r}\rangle\}$ representation and by $\langle\boldsymbol{p}|\psi\rangle = \tilde{\psi}(\boldsymbol{p})$ in the $\{|\boldsymbol{p}\rangle\}$ representation.

Therefore,

$$\psi(\boldsymbol{r}) = \langle\boldsymbol{r}|\psi\rangle = \int d^3p\ \langle\boldsymbol{r}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\psi\rangle = (2\pi\hbar)^{-3/2}\int d^3p\ e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}\tilde{\psi}(\boldsymbol{p}) \tag{1.105}$$

$$\tilde{\psi}(\boldsymbol{p}) = \langle\boldsymbol{p}|\psi\rangle = \int d^3r\ \langle\boldsymbol{p}|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\psi\rangle = (2\pi\hbar)^{-3/2}\int d^3r\ e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}\psi(\boldsymbol{r}) \tag{1.106}$$

$$A(\boldsymbol{p},\boldsymbol{p}') = (2\pi\hbar)^{-3}\int d^3r \int d^3r'\ e^{\frac{i}{\hbar}(\boldsymbol{p}\cdot\boldsymbol{r}-\boldsymbol{p}'\cdot\boldsymbol{r}')}A(\boldsymbol{r}',\boldsymbol{r}) \tag{1.107}$$

1.5.2 The R and P operators

We define the X, Y, Z operators whsoe action, in the $\{|\boldsymbol{r}\rangle\}$ representation, is given by:

$$\begin{array}{l} \langle\boldsymbol{r}|X|\psi\rangle = x\langle\boldsymbol{r}|\psi\rangle \\ \langle\boldsymbol{r}|Y|\psi\rangle = y\langle\boldsymbol{r}|\psi\rangle \\ \langle\boldsymbol{r}|Z|\psi\rangle = z\langle\boldsymbol{r}|\psi\rangle \end{array} \tag{1.108}$$

X, Y, and Z will be considered to be the components of a vector operator $\boldsymbol{R}$. Similarly, we define the vector operator $\boldsymbol{P}$ by its components P_x, P_y, P_z, whose action, in the $\{|\boldsymbol{p}\rangle\}$ representation is given by:

$$\begin{array}{l} \langle\boldsymbol{p}|P_x|\psi\rangle = p_x\langle\boldsymbol{p}|\psi\rangle \\ \langle\boldsymbol{p}|P_y|\psi\rangle = p_y\langle\boldsymbol{p}|\psi\rangle \\ \langle\boldsymbol{p}|P_z|\psi\rangle = p_z\langle\boldsymbol{p}|\psi\rangle \end{array} \tag{1.109}$$

How $\boldsymbol{P}$ operator acts in the $\{|\boldsymbol{r}\rangle\}$ representation? We use the closure relation to obtain:

$$\begin{aligned}
\langle \boldsymbol{r}|P_x|\psi\rangle &= \int d^3p\ \langle \boldsymbol{r}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|P_x|\psi\rangle \\
&\overset{(a)}{=} (2\pi\hbar)^{-3/2}\int d^3p\ e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}} p_x\tilde{\psi}(\boldsymbol{p}) \\
\langle \boldsymbol{r}|P_x|\psi\rangle &\overset{(b)}{=} \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(\boldsymbol{r}).
\end{aligned}$$

In (a) we have used the equation (1.104) while in (b) we have used the property of the derivative of a Fourier transform. Generally, the result is:

$$\boxed{\langle \boldsymbol{r}|\boldsymbol{P}|\psi\rangle = \frac{\hbar}{i}\nabla\langle \boldsymbol{r}|\psi\rangle = \frac{\hbar}{i}\nabla\psi(\boldsymbol{r})}\,. \tag{1.110}$$

In the $\{|bR\rangle\}$ representation, the $\boldsymbol{P}$ operator coincides with the differential operator $(\hbar/i)\nabla$ applied to the wave functions.

If we compute the commutator say, $[X, P_x]$, we have

$$\begin{aligned}
\langle \boldsymbol{r}|[X,P_x]|\psi\rangle &= \langle \boldsymbol{r}|(XP_x - P_xX)|\psi\rangle \\
&= \langle \boldsymbol{r}|XP_x|\psi\rangle - \langle \boldsymbol{r}|P_xX|\psi\rangle \\
&= \int d^3r'\ \langle \boldsymbol{r}|X|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|P_x|\psi\rangle - \int d^3r'\ \langle \boldsymbol{r}|P_x|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|X|\psi\rangle \\
&= \int d^3r'\ \left[x'\delta(\boldsymbol{r}-\boldsymbol{r}')\right]\frac{\hbar}{i}\frac{\partial}{\partial x}\langle \boldsymbol{r}'|\psi\rangle - \int d^3r'\ \left[\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(\boldsymbol{r}-\boldsymbol{r}')\right]x'\langle \boldsymbol{r}'|\psi\rangle \\
&= \frac{\hbar}{i}x\frac{\partial}{\partial x}\langle \boldsymbol{r}|\psi\rangle - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\langle \boldsymbol{r}|\psi\rangle) \\
&= \frac{\hbar}{i}x\frac{\partial}{\partial x}\langle \boldsymbol{r}|\psi\rangle - \frac{\hbar}{i}\langle \boldsymbol{r}|\psi\rangle - \frac{\hbar}{i}x\frac{\partial}{\partial x}\langle \boldsymbol{r}|\psi\rangle \\
\langle \boldsymbol{r}|[X,P_x]|\psi\rangle &= i\hbar\langle \boldsymbol{r}|\psi\rangle.
\end{aligned}$$

Thus, one finds $[X, P_x] = i\hbar$. In the same way, we find all the other commutators between the components of $\boldsymbol{R}$ and $\boldsymbol{P}$:

Canonical commutation relations $$\boxed{[R_i, R_j] = 0, \quad [P_i, P_j] = 0, \quad [R_i, P_j] = i\hbar\delta_{ij}, \quad i,j = 1,2,3}\,. \tag{1.111}$$

R and P are Hermitian

All the components of $\boldsymbol{R}$ and $\boldsymbol{P}$ are Hermitian operators.

For example,

$$\langle\varphi|X|\psi\rangle = \int d^3r\ \varphi^*(\boldsymbol{r})x\psi(\boldsymbol{r}) = \left[\int d^3r\ \varphi(\boldsymbol{r})x\psi^*(\boldsymbol{r})\right]^* = \langle\psi|X|\varphi\rangle^*.$$

Eigenvectors of R and P

Consider the action of X on the ket $|\boldsymbol{r}_0\rangle$:

$$\langle \boldsymbol{r}|X|\boldsymbol{r}_0\rangle = x\langle \boldsymbol{r}|\boldsymbol{r}_0\rangle = x\delta(\boldsymbol{r}-\boldsymbol{r}_0) = x_0\delta(\boldsymbol{r}-\boldsymbol{r}_0) = x_0\langle \boldsymbol{r}|\boldsymbol{r}_0\rangle.$$

The components in $\{|\boldsymbol{r}\rangle\}$ representation of the ket $X|\boldsymbol{r}_0\rangle$ are equal to those of the ket $\boldsymbol{r}_0$ multiplied by x_0:

$$X|\boldsymbol{r}_0\rangle = x_0|\boldsymbol{r}_0\rangle. \tag{1.112}$$

Omitting the index zero, and doing the same for the other components of $\boldsymbol{R}$ and $\boldsymbol{P}$ in their respective representations yield:

$$\begin{array}{l} X|\boldsymbol{r}\rangle = x|\boldsymbol{r}\rangle \\ Y|\boldsymbol{r}\rangle = y|\boldsymbol{r}\rangle \\ Z|\boldsymbol{r}\rangle = z|\boldsymbol{r}\rangle \end{array}, \quad \text{and} \quad \begin{array}{l} P_x|\boldsymbol{p}\rangle = p_x|\boldsymbol{p}\rangle \\ P_y|\boldsymbol{p}\rangle = p_y|\boldsymbol{p}\rangle \\ P_z|\boldsymbol{p}\rangle = p_z|\boldsymbol{p}\rangle \end{array} \tag{1.113}$$

R and P are observables

We have already demonstrated the closure relation for each representation $\{|\boldsymbol{r}\rangle\}$ and $\{|\boldsymbol{p}\rangle\}$ in equation (1.103). Therefore, $\boldsymbol{R}$ and $\boldsymbol{P}$ are observables. In a three-dimensional space, is necessary to specify the eigenvalues x_o, y_o, z_o as they uniquely determines the corresponding eigevector $|\boldsymbol{r}_0\rangle$.

> The set of the three operators X, Y, Z and the set of the three operators P_x, P_y, P_z constitute a CSCO in $\mathscr{E}_{\boldsymbol{r}}$.

Recall that an operator must have eigenvectors that span the whole state vector, so missing one coordinate will degenerate it and therefore is no longer uniquely determined. One can also mix X with P as $\{X, P_y, P_z\}$ to create CSCOs.

Formula sheet

Constants and Conversions

Unit	Name	Equivalent SI value
eV	electron-volt	$\approx 1.602 \cdot 10^{-19}\ J$
G	Gauss	$10^{-4}\ T$

Speed of light in vacuum	$c = 2.998 \cdot 10^{8}\ m/s$	Reduced Planck's constant	$\hbar = 1.055 \cdot 10^{-34}\ J \cdot s$

1.5.3 Useful formulas

Closure relation (discrete)	$\sum_k \sum_{i=1}^{g_k} \vert v_k^i\rangle\langle v_k^i\vert = \mathbb{1}$	Closure relation (continuous)	$\int_\beta d\beta\ \vert\omega_\beta\rangle\langle\omega_\beta\vert = \mathbb{1}$
Glauber Formula	$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$	Generalized uncertainty relation	$\Delta A \Delta B \geq \frac{1}{2}\vert\langle[A,B]\rangle\vert$
Function of an operator	$F(A) = \sum_{n=0}^{\infty} \frac{(A-a)^n}{n!} F^{(n)}(a)$		$\Delta Q = \sqrt{\langle Q^2\rangle - \langle Q\rangle^2}$
Transformation $\{u\} \to \{v\}$	$\mathbb{M}_{jk} = \langle u_j\vert v_k\rangle$	$\vert\psi\rangle_{\{u\}} = \mathbb{M}\vert\psi\rangle_{\{v\}}$ $A_{\{u\}} = \mathbb{M}A_{\{v\}}\mathbb{M}^\dagger$	$\vert\psi\rangle_{\{v\}} = \mathbb{M}^\dagger\vert\psi\rangle_{\{u\}}$ $A_{\{v\}} = \mathbb{M}^\dagger A_{\{u\}}\mathbb{M}$

1.5.4 Basis

Quantity	Discrete basis (sum over j, k)	Continuous basis (integrate over β, β')
$\mathbb{1}$	$= \sum \vert v_k\rangle\langle v_k\vert$	$= \int d\beta\ \vert\omega_\beta\rangle\langle\omega_\beta\vert$
$\vert\psi\rangle = \mathbb{1}\vert\psi\rangle$	$= \sum \vert v_k\rangle\langle v_k\vert\psi\rangle$	$= \int d\beta\ \vert\omega_\beta\rangle\langle\omega_\beta\vert\psi\rangle$
$\langle\varphi\vert = \langle\varphi\vert\mathbb{1}$	$= \sum \langle\varphi\vert v_k\rangle\langle v_k\vert$	$= \int d\beta\ \langle\varphi\vert\omega_\beta\rangle\langle\omega_\beta\vert$
$A = \mathbb{1}A\mathbb{1}$	$= \sum\sum \vert v_j\rangle\langle v_j\vert A\vert v_k\rangle\langle v_k\vert$	$= \iint d\beta\ d\beta'\ \vert\omega_\beta\rangle\langle\omega_\beta\vert A\vert\omega_{\beta'}\rangle\langle\omega_{\beta'}\vert$

Quantity	X representation	P_x representation
X	x	$i\hbar\,\partial/\partial p$
P_x	$-i\hbar\,\partial/\partial x$	p
$\vert x'\rangle$	$\langle x\vert x'\rangle = \delta(x-x')$	$\langle p\vert x'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(-ix'p/\hbar)$
$\vert p'\rangle$	$\langle x\vert p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(ixp'/\hbar)$	$\langle p\vert p'\rangle = \delta(p-p')$

Fourier transforms for 3D wavefunctions

$$\tilde{\psi}(\boldsymbol{p}) = \mathscr{F}[\psi(\boldsymbol{r})] = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\int_{-\infty}^{\infty} d^3\boldsymbol{r}\ e^{-i\boldsymbol{r}\cdot\boldsymbol{p}/\hbar}\psi(\boldsymbol{r}) \quad\Big|\quad \psi(\boldsymbol{r}) = \mathscr{F}^{-1}\left[\tilde{\psi}(\boldsymbol{p})\right] = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\int_{-\infty}^{\infty} d^3\boldsymbol{p}\ e^{i\boldsymbol{r}\cdot\boldsymbol{p}/\hbar}\tilde{\psi}(\boldsymbol{p})$$

Commutators

$[A, B] = -[B, A]$ $\quad$ $[A + B, C + D] = [A, C] + [A, D] + [B, C] + [B, D]$
$e^{A+B} = e^{A}e^{B}e^{\frac{1}{2}[A,B]}$

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