where $\overline{V}(\mathbf{p})$ is the Fourier transform of $V(\mathbf{r})$:

$$\overline{V}(\mathbf{p}) = (2\pi\hbar)^{-3/2} \int d^3r \, e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} \, V(\mathbf{r}) \tag{31}$$

The Schrödinger equation in the $\{ \mid \mathbf{p} \rangle \}$ representation is therefore written:

$$i\hbar \frac{\partial}{\partial t} \overline{\psi}(\mathbf{p}, t) = \frac{\mathbf{p}^2}{2m} \overline{\psi}(\mathbf{p}, t) + (2\pi\hbar)^{-3/2} \int d^3p' \, \overline{V}(\mathbf{p} - \mathbf{p}') \overline{\psi}(\mathbf{p}', t) \tag{32}$$

COMMENT:

Since $\overline{\psi}(\mathbf{p}, t)$ is the Fourier transform of $\psi(\mathbf{r}, t)$ [*cf.* formula (E-18) of chapter II], it would have been possible to find equation (32) by taking the Fourier transforms of both sides of equation (19).





## Complement $E_{II}$

# SOME GENERAL PROPERTIES OF TWO OBSERVABLES, $Q$ AND $P$, WHOSE COMMUTATOR IS EQUAL TO $i\hbar$



In quantum mechanics, one often encounters operators whose commutator is equal to $i\hbar$. This is the case, for example, when these two operators correspond to the two classical conjugate quantities $q_i$ and $p_i$ $\left(q_i\text{, the coordinate in a system of orthonormal axes, and the conjugate momentum } p_i = \frac{\partial \mathscr{L}}{\partial \dot{q}_i}\right)$. In quantum mechanics, one associates with $q_i$ and $p_i$ the operators $Q_i$ and $P_i$ which satisfy the relation:

$$[Q_i, P_i] = i\hbar \tag{1}$$

In § E of chapter II, we encountered such operators: $X$ and $P_x$. In this complement, we shall take a more general point of view and show that it is possible to establish a whole series of important properties relative to two observables $P$ and $Q$ whose commutator is equal to $i\hbar$. All these properties are consequences of commutation relation (1).

## 1. The operator $S(\lambda)$: definition, properties

We shall consider two observables $P$ and $Q$, satisfying the relation:

$$[Q, P] = i\hbar \tag{2}$$

and we shall define the operator $S(\lambda)$, which depends on the real parameter $\lambda$, by:

$$S(\lambda) = e^{-i\lambda P/\hbar} \tag{3}$$

This operator is unitary; it is easy to verify the relations:

$$S^\dagger(\lambda) = S^{-1}(\lambda) = S(-\lambda) \tag{4}$$

Let us calculate the commutator $[Q, S(\lambda)]$. We can apply formula (51) of complement $B_{II}$, since $[Q, P] = i\hbar$ commutes with $Q$ and $P$:

$$[Q, S(\lambda)] = i\hbar\left(-\frac{i\lambda}{\hbar}\right) e^{-i\lambda P/\hbar} = \lambda S(\lambda) \tag{5}$$

This relation can also be written:

$$Q S(\lambda) = S(\lambda)[Q + \lambda] \tag{6}$$

Finally, note that:

$$S(\lambda) S(\mu) = S(\lambda + \mu) \tag{7}$$

## 2. Eigenvalues and eigenvectors of Q

### a. SPECTRUM OF Q

Assume that $Q$ has a non-zero eigenvector $|\, q \rangle$, with eigenvalue $q$:

$$Q \,|\, q \rangle = q \,|\, q \rangle \tag{8}$$

Apply equation (6) to the vector $|\, q \rangle$. This yields:

$$\begin{aligned} Q\ S(\lambda) \,|\, q \rangle &= S(\lambda)(Q + \lambda) \,|\, q \rangle \\ &= S(\lambda)(q + \lambda) \,|\, q \rangle = (q + \lambda)\, S(\lambda) \,|\, q \rangle \end{aligned} \tag{9}$$

This equation expresses the fact that $S(\lambda) \,|\, q \rangle$ is another non-zero eigenvector of $Q$, with an eigenvalue of $(q + \lambda)$ ($S(\lambda) \,|\, q \rangle$ is non-zero because $S(\lambda)$ is unitary). Thus, starting with an eigenvector of $Q$, one can, by applying $S(\lambda)$, construct another eigenvector of $Q$, with any real eigenvalue ($\lambda$ can indeed take on any real value). The spectrum of $Q$ is therefore a continuous spectrum, composed of all possible values on the real axis*.

### b. DEGREE OF DEGENERACY

From now on, we shall assume, for simplicity, that the eigenvalue $q$ of $Q$ is non-degenerate (the results which we shall derive can be generalized to the case where $q$ is degenerate). Let us show that if $q$ is non-degenerate, all the other eigenvalues of $Q$ are also non-degenerate. Let us assume, for example, that the eigenvalue $q + \lambda$ is two-fold degenerate, and we shall show that we arrive at a contradiction. There would then exist two orthogonal eigenvectors, $|\, q + \lambda, \alpha \rangle$ and $|\, q + \lambda, \beta \rangle$, corresponding to the eigenvalue $q + \lambda$:

$$\langle q + \lambda, \beta \,|\, q + \lambda, \alpha \rangle = 0 \tag{10}$$

Consider the two vectors $S(-\lambda) \,|\, q + \lambda, \alpha \rangle$ and $S(-\lambda) \,|\, q + \lambda, \beta \rangle$. They are, according to (9), two eigenvectors of $Q$, with an eigenvalue of $q + \lambda - \lambda = q$. They are not collinear, since they are orthogonal; their scalar product can be written, using the fact that $S(\lambda)$ is unitary:

$$\langle q + \lambda, \beta \,|\, S^{\dagger}(-\lambda) S(-\lambda) \,|\, q + \lambda, \alpha \rangle = \langle q + \lambda, \beta \,|\, q + \lambda, \alpha \rangle = 0 \tag{11}$$

We reach the conclusion that $q$ is at least two-fold degenerate, which is contrary to the initial hypothesis. Consequently, all the eigenvalues of $Q$ must have the same degree of degeneracy.

### c. EIGENVECTORS

We shall fix the relative phases of the different eigenvectors of $Q$ with respect to the eigenvector $|\, 0 \rangle$, of eigenvalue 0, by setting:

$$|\, q \rangle = S(q) \,|\, 0 \rangle \tag{12}$$

Applying $S(\lambda)$ to both sides of (12) and using (7), we obtain:

$$S(\lambda) \,|\, q \rangle = S(\lambda) S(q) \,|\, 0 \rangle = S(\lambda + q) \,|\, 0 \rangle = |\, q + \lambda \rangle \tag{13}$$

The adjoint expression of (13) is written:

$$\langle q \,|\, S^{\dagger}(\lambda) = \langle q + \lambda \,| \tag{14}$$

or, using (4) and replacing $\lambda$ by $-\lambda$:

$$\langle q \,|\, S(\lambda) = \langle q - \lambda \,| \tag{15}$$

## 3. The $\{ |\, q \rangle \}$ representation

Since $Q$ is an observable, the set of its eigenvectors $\{ |\, q \rangle \}$ constitutes a basis of $\mathscr{E}$. It is possible to characterize each ket by its "wave function in the $\{ |\, q \rangle \}$ representation":

$$\psi(q) = \langle q \,|\, \psi \rangle \tag{16}$$

### a. THE ACTION OF Q IN THE $\{ |\, q \rangle \}$ REPRESENTATION

Let us calculate in the $\{ |\, q \rangle \}$ representation the wave function associated with the ket $Q \,|\, \psi \rangle$. It is written:

$$\langle q \,|\, Q \,|\, \psi \rangle = q \langle q \,|\, \psi \rangle = q\psi(q) \tag{17}$$

[using (8) and the fact that $Q$ is Hermitian]. The action of $Q$ in the $\{ |\, q \rangle \}$ representation is therefore simply a multiplication by $q$.

* This shows that in a space $\mathscr{E}$ of finite dimension $N$, there are no observables $Q$ and $P$, whose commutator is equal to $i\hbar$. The number of eigenvalues of $Q$ could not be simultaneously less than or equal to $N$ and infinite.

This result can be derived directly, moreover, by taking the trace of relation (2): $\text{Tr}\, QP - \text{Tr}\, PQ = \text{Tr}\, i\hbar$. When $N$ is finite, the traces on the left-hand side of this equation exist: they are finite and equal numbers [*cf.* complement $B_{II}$, formula (7-a)]. The equation becomes $0 = \text{Tr}\, i\hbar = Ni\hbar$, which is impossible.

### b. THE ACTION OF $S(\lambda)$ IN THE $\{ | q \rangle \}$ REPRESENTATION ; THE TRANSLATION OPERATOR

The wave function in the $\{ | q \rangle \}$ representation associated with the ket $S(\lambda) | \psi \rangle$ is written [formula (15)]:

$$\langle q | S(\lambda) | \psi \rangle = \langle q - \lambda | \psi \rangle = \psi(q - \lambda) \tag{18}$$

The action of the operator $S(\lambda)$ in the $\{ | q \rangle \}$ representation is therefore a translation of the wave function over a distance $\lambda$ parallel to the $q$-axis*. For this reason, $S(\lambda)$ is called the *translation operator*.

### c. THE ACTION OF P IN THE $\{ | q \rangle \}$ REPRESENTATION

When $\varepsilon$ is an infinitely small quantity, we have:

$$S(-\varepsilon) = e^{i\varepsilon P/\hbar} = \mathbb{1} + i\frac{\varepsilon}{\hbar} P + O(\varepsilon^2) \tag{19}$$

Consequently :

$$\langle q | S(-\varepsilon) | \psi \rangle = \psi(q) + i\frac{\varepsilon}{\hbar} \langle q | P | \psi \rangle + O(\varepsilon^2) \tag{20}$$

On the other hand, equation (18) yields:

$$\langle q | S(-\varepsilon) | \psi \rangle = \psi(q + \varepsilon) \tag{21}$$

Comparison of (20) and (21) shows that:

$$\psi(q + \varepsilon) = \psi(q) + i\frac{\varepsilon}{\hbar} \langle q | P | \psi \rangle + O(\varepsilon^2) \tag{22}$$

It follows that:

$$\langle q | P | \psi \rangle = \frac{\hbar}{i} \lim_{\varepsilon \to 0} \frac{\psi(q + \varepsilon) - \psi(q)}{\varepsilon}$$
$$= \frac{\hbar}{i} \frac{d}{dq} \psi(q) \tag{23}$$

The action of $P$ in the $\{ | q \rangle \}$ representation is therefore that of $\frac{\hbar}{i}\frac{d}{dq}$. Equation (E-26) of chapter II is thus generalized.

## 4. The $\{ | p \rangle \}$ representation. The symmetrical nature of the $P$ and $Q$ observables

Relation (23) enables us to obtain easily the wave function $v_p(q)$ associated, in the $\{ | q \rangle \}$ representation, with the eigenvector $| p \rangle$ of $P$ with an eigenvalue of $p$ :

$$v_p(q) = \langle q | p \rangle = (2\pi\hbar)^{-1/2} e^{\frac{i}{\hbar} pq} \tag{24}$$

* The function $f(x - a)$ is the function which, at the point $x = x_0 + a$, takes on the value $f(x_0)$. It is therefore the function obtained from $f(x)$ by a translation of $+ a$.





We can therefore write :

$$| p \rangle = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} dq \, e^{\frac{i}{\hbar} pq} | q \rangle \tag{25}$$

A ket $| \psi \rangle$ can be defined by its "wave function in the $\{ | p \rangle \}$ representation":

$$\overline{\psi}(p) = \langle p | \psi \rangle \tag{26}$$

Using the adjoint relation of (25), we obtain:

$$\overline{\psi}(p) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} dq \, e^{-\frac{i}{\hbar} pq} \psi(q) \tag{27}$$

$\overline{\psi}(p)$ is therefore the Fourier transform of $\psi(q)$.

The action of the $P$ operator in the $\{ | p \rangle \}$ representation corresponds to a multiplication by $p$; that of the $Q$ operator corresponds, as can easily be shown using (27), to the operation $i\hbar \frac{d}{dp}$.

Thus we obtain symmetrical results in the $\{ | q \rangle \}$ and $\{ | p \rangle \}$ representations. This is not surprising : in our hypotheses, it is possible to exchange the $P$ and $Q$ operators, simply changing the sign of the commutator in relation (2). Instead of introducing the operator $S(\lambda)$, we could therefore have considered $T(\lambda')$ defined by:

$$T(\lambda') = e^{i\lambda' Q/\hbar} \tag{28}$$

and we could have developed the same arguments, replacing $P$ by $Q$ and $i$ by $-i$ everywhere.

References:

Messiah (1.17), Vol. I, § VIII-6; Dirac (1.13), § 25; Merzbacher (1.16), chap. 14, § 7.

(to within multiplicative factors). Specifying a possible set of eigenvalues $\{ a_n, b_p, c_r \}$ of $A$, $B$, $C$ then characterizes only one of the vectors of this basis. If this is not the case, one adds to $A$, $B$, $C$ an observable $D$ which commutes with each of these three operators, and so on. In general, we are thus led to the following:

*By definition, a set of observables A, B, C... is called a complete set of commuting observables if*

*(i) all the observables A, B, C... commute by pairs,*

*(ii) specifying the eigenvalues of all the operators A, B, C... determines a unique* (to within a multiplicative factor) *common eigenvector.*

An equivalent way of saying this is the following:

*A set of observables A, B, C... is a complete set of commuting observables if there exists a unique orthonormal basis of common eigenvectors* (to within phase factors).

C.S.C.O.'s play an important role in quantum mechanics. We shall see numerous examples of them (see, in particular, § E-2-d).

COMMENTS:

(*i*) If $\{ A, B \}$ is a C.S.C.O., another C.S.C.O. can be obtained by adding to it any observable $C$, on the condition, of course, that it commutes with $A$ and $B$. However, it is generally understood that one is confined to "minimal" sets, that is, those which cease to be complete when any one of the observables is omitted.

(*ii*) Let $\{ A, B, C \}$ be a complete set of commuting observables. Since the specification of the eigenvalues $a_n$, $b_p$, $c_r$... determines a ket of the corresponding basis (to within a constant factor), this ket is sometimes denoted by $| a_n, b_p, c_r, ... \rangle$.

(*iii*) For a given physical system, there exist several complete sets of commuting observables. We shall see a particular example of this in § E-2-d.

# E. TWO IMPORTANT EXAMPLES OF REPRESENTATIONS AND OBSERVABLES

In this paragraph, we shall return to the $\mathscr{F}$-space of wave functions of a particle, or, more exactly, to the state space $\mathscr{E}_r$ which is associated with it and which we shall define in the following way. Let there correspond to every wave function $\psi(\mathbf{r})$ a ket $| \psi \rangle$ belonging to $\mathscr{E}_r$; this correspondence is linear. Moreover, the scalar product of two kets coincides with that of the functions which are associated with them:

$$\langle \varphi | \psi \rangle = \int d^3r \; \varphi^*(\mathbf{r}) \; \psi(\mathbf{r}) \tag{E-1}$$





$\mathscr{E}_r$ is thus the state space of a (spinless) particle.

We are going to define and study, in this space, two representations and two operators which are particularly important. In chapter III we shall associate them with the position and the momentum of the particle under consideration. They will enable us, moreover, to apply and illustrate the concepts which we have introduced in the preceding sections.

## 1. The $\{ | \mathbf{r} \rangle \}$ and $\{ | \mathbf{p} \rangle \}$ representations

### a. DEFINITION

In §§ A-3-a and A-3-b, we introduced two particular "bases" of $\mathscr{F}$: $\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$ and $\{ v_{\mathbf{p}_0}(\mathbf{r}) \}$. They are not composed of functions belonging to $\mathscr{F}$:

$$\xi_{\mathbf{r}_0}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_0) \tag{E-2-a}$$

$$v_{\mathbf{p}_0}(\mathbf{r}) = (2\pi\hbar)^{-3/2} \, e^{\frac{i}{\hbar}\mathbf{p}_0 \cdot \mathbf{r}} \tag{E-2-b}$$

However, every sufficiently regular square-integrable function can be expanded in one or the other of these "bases".

This is why we shall remove the quotation marks and associate a ket with each of the functions of these bases (*cf.* § B-2-c). The ket associated with $\xi_{\mathbf{r}_0}(\mathbf{r})$ will be denoted simply by $| \mathbf{r}_0 \rangle$, and that associated with $v_{\mathbf{p}_0}(\mathbf{r})$, by $| \mathbf{p}_0 \rangle$:

$$\xi_{\mathbf{r}_0}(\mathbf{r}) \iff | \mathbf{r}_0 \rangle \tag{E-3-a}$$

$$v_{\mathbf{p}_0}(\mathbf{r}) \iff | \mathbf{p}_0 \rangle \tag{E-3-b}$$

Using the bases $\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$ and $\{ v_{\mathbf{p}_0}(\mathbf{r}) \}$ of $\mathscr{F}$, we thus define in $\mathscr{E}_r$ two representations: the $\{ | \mathbf{r}_0 \rangle \}$ representation and the $\{ | \mathbf{p}_0 \rangle \}$ representation. A basis vector of the first one is characterized by three "continuous indices" $x_0$, $y_0$ and $z_0$, which are the coordinates of a point in three-dimensional space; for the second, the three indices are also the components of an ordinary vector.

### b. ORTHONORMALIZATION AND CLOSURE RELATIONS

Let us calculate $\langle \mathbf{r}_0 | \mathbf{r}'_0 \rangle$. Using the definition of the scalar product in $\mathscr{E}_r$:

$$\langle \mathbf{r}_0 | \mathbf{r}'_0 \rangle = \int d^3r \; \xi^*_{\mathbf{r}_0}(\mathbf{r}) \; \xi_{\mathbf{r}'_0}(\mathbf{r}) = \delta(\mathbf{r}_0 - \mathbf{r}'_0) \tag{E-4-a}$$

where relation (A-55) has been used. In the same way:

$$\langle \mathbf{p}_0 | \mathbf{p}'_0 \rangle = \int d^3r \; v^*_{\mathbf{p}_0}(\mathbf{r}) \; v_{\mathbf{p}'_0}(\mathbf{r}) = \delta(\mathbf{p}_0 - \mathbf{p}'_0) \tag{E-4-b}$$

using (A-47). The bases which we have just defined are therefore orthonormal in the extended sense.

The fact that the set of the $|\mathbf{r}_0\rangle$ or that of the $|\mathbf{p}_0\rangle$ constitutes a basis in $\mathscr{E}_\mathbf{r}$ can be expressed by a closure relation in $\mathscr{E}_\mathbf{r}$. This is written in an analogous manner to (C-10), integrating here, however, over three indices instead of one.

We therefore have the fundamental relations:

$$\begin{array}{|ll|ll|} \hline \langle \mathbf{r}_0 | \mathbf{r}'_0 \rangle = \delta(\mathbf{r}_0 - \mathbf{r}'_0) & \text{(a)} & \langle \mathbf{p}_0 | \mathbf{p}'_0 \rangle = \delta(\mathbf{p}_0 - \mathbf{p}'_0) & \text{(c)} \\ \int d^3r_0\, |\mathbf{r}_0\rangle\langle \mathbf{r}_0| = \mathbb{1} & \text{(b)} & \int d^3p_0\, |\mathbf{p}_0\rangle\langle \mathbf{p}_0| = \mathbb{1} & \text{(d)} \\ \hline \end{array} \qquad \text{(E-5)}$$

## c. COMPONENTS OF A KET

Consider an arbitrary ket $|\psi\rangle$, corresponding to the wave function $\psi(\mathbf{r})$. The preceding closure relations enable us to write it in either of these two forms:

$$|\psi\rangle = \int d^3r_0\, |\mathbf{r}_0\rangle\langle \mathbf{r}_0|\psi\rangle \qquad \text{(E-6-a)}$$

$$|\psi\rangle = \int d^3p_0\, |\mathbf{p}_0\rangle\langle \mathbf{p}_0|\psi\rangle \qquad \text{(E-6-b)}$$

The coefficients $\langle \mathbf{r}_0|\psi\rangle$ and $\langle \mathbf{p}_0|\psi\rangle$ can be calculated using the formulas:

$$\langle \mathbf{r}_0|\psi\rangle = \int d^3r\; \xi^*_{\mathbf{r}_0}(\mathbf{r})\; \psi(\mathbf{r}) \qquad \text{(E-7-a)}$$

$$\langle \mathbf{p}_0|\psi\rangle = \int d^3r\; v^*_{\mathbf{p}_0}(\mathbf{r})\; \psi(\mathbf{r}) \qquad \text{(E-7-b)}$$

We then find:

$$\boxed{\begin{aligned} \langle \mathbf{r}_0|\psi\rangle &= \psi(\mathbf{r}_0) \\ \langle \mathbf{p}_0|\psi\rangle &= \overline{\psi}(\mathbf{p}_0) \end{aligned}} \qquad \begin{aligned} &\text{(E-8-a)} \\ &\text{(E-8-b)} \end{aligned}$$

where $\overline{\psi}(\mathbf{p})$ is the Fourier transform of $\psi(\mathbf{r})$.

*The value $\psi(\mathbf{r}_0)$ of the wave function at the point $\mathbf{r}_0$ is thus shown to be the component of the ket $|\psi\rangle$ on the basis vector $|\mathbf{r}_0\rangle$ of the $\{|\mathbf{r}_0\rangle\}$ representation.* The "wave function in momentum space" $\overline{\psi}(\mathbf{p})$ can be interpreted analogously. The possibility of characterizing $|\psi\rangle$ by $\psi(\mathbf{r})$ is thus simply a special case of the results of § C-3-a.

For example, for $|\psi\rangle = |\mathbf{p}_0\rangle$, formula (E-8-a) gives:

$$\langle \mathbf{r}_0|\mathbf{p}_0\rangle = v_{\mathbf{p}_0}(\mathbf{r}_0) = (2\pi\hbar)^{-3/2}\, e^{\frac{i}{\hbar}\mathbf{p}_0\cdot\mathbf{r}_0} \qquad \text{(E-9)}$$





For $|\psi\rangle = |\mathbf{r}'_0\rangle$, the result is indeed in agreement with the orthonormalization relation (E-5-a):

$$\langle \mathbf{r}_0|\mathbf{r}'_0\rangle = \xi_{\mathbf{r}'_0}(\mathbf{r}_0) = \delta(\mathbf{r}_0 - \mathbf{r}'_0) \qquad \text{(E-10)}$$

Now that we have reinterpreted the wave function $\psi(\mathbf{r})$ and its Fourier transform $\overline{\psi}(\mathbf{p})$, we shall denote the basis vectors of the two representations we are studying here by $|\mathbf{r}\rangle$ and $|\mathbf{p}\rangle$, instead of $|\mathbf{r}_0\rangle$ and $|\mathbf{p}_0\rangle$. Formulas (E-8) can then be written:

$$\langle \mathbf{r}|\psi\rangle = \psi(\mathbf{r}) \qquad \text{(E-8-a)}$$

$$\langle \mathbf{p}|\psi\rangle = \overline{\psi}(\mathbf{p}) \qquad \text{(E-8-b)}$$

and the orthonormalization and closure relations (E-5) become:

$$\begin{array}{llll} \langle \mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') & \text{(a)} & \langle \mathbf{p}|\mathbf{p}'\rangle = \delta(\mathbf{p}-\mathbf{p}') & \text{(c)} \\ \int d^3r\, |\mathbf{r}\rangle\langle \mathbf{r}| = \mathbb{1} & \text{(b)} & \int d^3p\, |\mathbf{p}\rangle\langle \mathbf{p}| = \mathbb{1} & \text{(d)} \end{array} \qquad \text{(E-5)}$$

Of course, $\mathbf{r}$ and $\mathbf{p}$ are still considered to represent two sets of *continuous indices*, $\{x, y, z\}$ and $\{p_x, p_y, p_z\}$, which fix the basis kets of the $\{|\mathbf{r}\rangle\}$ and $\{|\mathbf{p}\rangle\}$ representations respectively.

Now let $\{u_i(\mathbf{r})\}$ be an orthonormal basis of $\mathscr{F}$. With each $u_i(\mathbf{r})$ is associated a ket $|u_i\rangle$ of $\mathscr{E}_\mathbf{r}$. The set $\{|u_i\rangle\}$ forms an orthonormal basis in $\mathscr{E}_\mathbf{r}$; it therefore satisfies the closure relation:

$$\sum_i |u_i\rangle\langle u_i| = \mathbb{1} \qquad \text{(E-11)}$$

Evaluate the matrix element of both sides of (E-11) between $|\mathbf{r}\rangle$ and $|\mathbf{r}'\rangle$:

$$\sum_i \langle \mathbf{r}|u_i\rangle\langle u_i|\mathbf{r}'\rangle = \langle \mathbf{r}|\mathbb{1}|\mathbf{r}'\rangle = \langle \mathbf{r}|\mathbf{r}'\rangle \qquad \text{(E-12)}$$

According to (E-8-a) and (E-5-a), this relation can be written:

$$\sum_i u_i(\mathbf{r})\; u_i^*(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \qquad \text{(E-13)}$$

The closure relation for the $\{u_i(\mathbf{r})\}$ [formula (A-32)] is therefore simply the expression in the $\{|\mathbf{r}\rangle\}$ representation of the vectorial closure relation (E-11).

## d. THE SCALAR PRODUCT OF TWO VECTORS

We have defined the scalar product of two kets of $\mathscr{E}_\mathbf{r}$ as being equal to that of the associated wave functions in $\mathscr{F}$ [equation (E-1)]. In light of the discussion in § c, this definition appears simply as a special case of formula (C-21). (E-1) can, in fact, be derived by inserting the closure relation (E-5-b) between $\langle\varphi|$ and $|\psi\rangle$:

$$\langle \varphi|\psi\rangle = \int d^3r\, \langle \varphi|\mathbf{r}\rangle\langle \mathbf{r}|\psi\rangle \qquad \text{(E-14)}$$

and by interpreting the components $\langle \mathbf{r} | \psi \rangle$ and $\langle \mathbf{r} | \varphi \rangle$ as in (E-8-a).

If we place ourselves in the $\{ | \mathbf{p} \rangle \}$ representation, a well-known property of the Fourier transform is demonstrated (appendix I, § 2-c).

$$\langle \varphi | \psi \rangle = \int d^3p \, \langle \varphi | \mathbf{p} \rangle \langle \mathbf{p} | \psi \rangle = \int d^3p \; \bar{\varphi}^*(\mathbf{p}) \; \bar{\psi}(\mathbf{p}) \tag{E-15}$$

### e. CHANGING FROM THE $\{ | \mathbf{r} \rangle \}$ REPRESENTATION TO THE $\{ | \mathbf{p} \rangle \}$ REPRESENTATION

This is accomplished using the method indicated in § C-5, the only difference arising from the fact that we are dealing here with two continuous bases. Changing from one basis to the other brings in the numbers :

$$\langle \mathbf{r} | \mathbf{p} \rangle = \langle \mathbf{p} | \mathbf{r} \rangle^* = (2\pi\hbar)^{-3/2} \, e^{\frac{i}{\hbar}\mathbf{p}.\mathbf{r}} \tag{E-16}$$

A given ket $| \psi \rangle$ is represented by $\langle \mathbf{r} | \psi \rangle = \psi(\mathbf{r})$ in the $\{ | \mathbf{r} \rangle \}$ representation and by $\langle \mathbf{p} | \psi \rangle = \bar{\psi}(\mathbf{p})$ in the $\{ | \mathbf{p} \rangle \}$ representation. We already know [formula (E-7-b)] that $\psi(\mathbf{r})$ and $\bar{\psi}(\mathbf{p})$ are related by a Fourier transform. This is indeed what the formulas for the representation change yield:

$$\langle \mathbf{r} | \psi \rangle = \int d^3p \, \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{p} | \psi \rangle$$

that is:

$$\psi(\mathbf{r}) = (2\pi\hbar)^{-3/2} \int d^3p \; e^{\frac{i}{\hbar}\mathbf{p}.\mathbf{r}} \; \bar{\psi}(\mathbf{p}) \tag{E-17}$$

Inversely:

$$\langle \mathbf{p} | \psi \rangle = \int d^3r \, \langle \mathbf{p} | \mathbf{r} \rangle \langle \mathbf{r} | \psi \rangle$$

that is:

$$\bar{\psi}(\mathbf{p}) = (2\pi\hbar)^{-3/2} \int d^3r \; e^{-\frac{i}{\hbar}\mathbf{p}.\mathbf{r}} \; \psi(\mathbf{r}) \tag{E-18}$$

By applying the general formula (C-56), one can easily pass from the matrix elements $\langle \mathbf{r}' | A | \mathbf{r} \rangle = A(\mathbf{r}', \mathbf{r})$ of an operator $A$ in the $\{ | \mathbf{r} \rangle \}$ representation to the matrix elements $\langle \mathbf{p}' | A | \mathbf{p} \rangle = A(\mathbf{p}', \mathbf{p})$ of the same operator in the $\{ | \mathbf{p} \rangle \}$ representation:

$$A(\mathbf{p}', \mathbf{p}) = (2\pi\hbar)^{-3} \int d^3r \int d^3r' \; e^{\frac{i}{\hbar}(\mathbf{p}.\mathbf{r} - \mathbf{p}'.\mathbf{r}')} \; A(\mathbf{r}', \mathbf{r}) \tag{E-19}$$

An analogous formula enables one to calculate $A(\mathbf{r}', \mathbf{r})$ from $A(\mathbf{p}', \mathbf{p})$.





## 2. The R and P operators

### a. DEFINITION

Let $| \psi \rangle$ be an arbitrary ket of $\mathscr{E}_\mathbf{r}$ and let $\langle \mathbf{r} | \psi \rangle = \psi(\mathbf{r}) \equiv \psi(x, y, z)$ be the corresponding wave function. Using the definition of the operator $X$, the ket:

$$| \psi' \rangle = X | \psi \rangle \tag{E-20}$$

is represented, in the $\{ | \mathbf{r} \rangle \}$ basis, by the function $\langle \mathbf{r} | \psi' \rangle = \psi'(\mathbf{r}) \equiv \psi'(x, y, z)$ such that:

$$\psi'(x, y, z) = x \; \psi(x, y, z) \tag{E-21}$$

In the $\{ | \mathbf{r} \rangle \}$ representation, the $X$ operator therefore coincides with the operator which multiplies by $x$. Although we characterize $X$ by the way in which it transforms the wave functions, it is an operator which acts in the state space $\mathscr{E}_\mathbf{r}$. We can introduce two other operators, $Y$ and $Z$, in an analogous manner. Thus we define $X$, $Y$ and $Z$ by the formulas:

$$\langle \mathbf{r} | X | \psi \rangle = x \langle \mathbf{r} | \psi \rangle \tag{E-22-a}$$
$$\langle \mathbf{r} | Y | \psi \rangle = y \langle \mathbf{r} | \psi \rangle \tag{E-22-b}$$
$$\langle \mathbf{r} | Z | \psi \rangle = z \langle \mathbf{r} | \psi \rangle \tag{E-22-c}$$

where the numbers $x$, $y$, $z$ are precisely the three indices which label the ket $| \mathbf{r} \rangle$. $X$, $Y$ and $Z$ will be considered to be the "components" of a "vector operator" $\mathbf{R}$: for the moment, we shall treat this simply as a condensed notation, suggested by the fact that $x$, $y$, $z$ are the components of the ordinary vector $\mathbf{r}$.

Manipulation of the $X$, $Y$, $Z$ operators is particularly simple in the $\{ | \mathbf{r} \rangle \}$ representation. For example, in order to calculate the matrix element $\langle \varphi | X | \psi \rangle$, all we need to do is insert the closure relation (E-5-b) between $\langle \varphi |$ and $X$ and use definition (E-22):

$$\langle \varphi | X | \psi \rangle = \int d^3r \, \langle \varphi | \mathbf{r} \rangle \langle \mathbf{r} | X | \psi \rangle = \int d^3r \; \varphi^*(\mathbf{r}) \; x \; \psi(\mathbf{r}) \tag{E-23}$$

Similarly, we define the vector operator $\mathbf{P}$ by its components $P_x$, $P_y$, $P_z$, whose action, in the $\{ | \mathbf{p} \rangle \}$ representation, is given by:

$$\langle \mathbf{p} | P_x | \psi \rangle = p_x \langle \mathbf{p} | \psi \rangle \tag{E-24-a}$$
$$\langle \mathbf{p} | P_y | \psi \rangle = p_y \langle \mathbf{p} | \psi \rangle \tag{E-24-b}$$
$$\langle \mathbf{p} | P_z | \psi \rangle = p_z \langle \mathbf{p} | \psi \rangle \tag{E-24-c}$$

where $p_x$, $p_y$, $p_z$ are the three indices which appear in the ket $| \mathbf{p} \rangle$.

Let us ascertain how the $\mathbf{P}$ operator acts in the $\{ | \mathbf{r} \rangle \}$ representation.

To do so (*cf.* §C-5-d), we use the closure relation (E-5-d) and the transformation matrix (E-16) to obtain:

$$\langle \mathbf{r} | P_x | \psi \rangle = \int d^3p \, \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{p} | P_x | \psi \rangle$$

$$= (2\pi\hbar)^{-3/2} \int d^3p \; e^{\frac{i}{\hbar}\mathbf{p}.\mathbf{r}} \; p_x \; \bar{\psi}(\mathbf{p}) \qquad \text{(E-25)}$$

We recognize in (E-25) the Fourier transform of $p_x\bar{\psi}(\mathbf{p})$, that is $\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(\mathbf{r})$ [appendix I, relation (38-a)]. Therefore:

$$\langle \mathbf{r} | \mathbf{P} | \psi \rangle = \frac{\hbar}{i} \nabla \langle \mathbf{r} | \psi \rangle \qquad \text{(E-26)}$$

In the $\{ | \mathbf{r} \rangle \}$ representation, the **P** operator coincides with the differential operator $\frac{\hbar}{i}\nabla$ applied to the wave functions. The calculation of a matrix element such as $\langle \varphi | P_x | \psi \rangle$ in the $\{ | \mathbf{r} \rangle \}$ representation is therefore performed in the following manner:

$$\langle \varphi | P_x | \psi \rangle = \int d^3r \, \langle \varphi | \mathbf{r} \rangle \langle \mathbf{r} | P_x | \psi \rangle$$

$$= \int d^3r \; \varphi^*(\mathbf{r}) \left[ \frac{\hbar}{i} \frac{\partial}{\partial x} \right] \psi(\mathbf{r}) \qquad \text{(E-27)}$$

Placing ourselves in the $\{ | \mathbf{r} \rangle \}$ representation, we can also calculate the commutators between the $X$, $Y$, $Z$, $P_x$, $P_y$, $P_z$ operators. For example:

$$\langle \mathbf{r} | [X, P_x] | \psi \rangle = \langle \mathbf{r} | (XP_x - P_xX) | \psi \rangle$$

$$= x \langle \mathbf{r} | P_x | \psi \rangle - \frac{\hbar}{i}\frac{\partial}{\partial x} \langle \mathbf{r} | X | \psi \rangle$$

$$= \frac{\hbar}{i} x \frac{\partial}{\partial x} \langle \mathbf{r} | \psi \rangle - \frac{\hbar}{i}\frac{\partial}{\partial x} x \langle \mathbf{r} | \psi \rangle$$

$$= i\hbar \langle \mathbf{r} | \psi \rangle \qquad \text{(E-28)}$$

This calculation is valid for all $| \psi \rangle$ and for any ket of the $| \mathbf{r} \rangle$ basis. Thus one finds*:

$$[X, P_x] = i\hbar \qquad \text{(E-29)}$$

In the same way, we find all the other commutators between the components of **R** and those of **P**. The result can be written in the form:

$$\left. \begin{array}{l} [R_i, R_j] = 0 \\ [P_i, P_j] = 0 \\ [R_i, P_j] = i\hbar\delta_{ij} \end{array} \right\} i, j = 1, 2, 3 \qquad \text{(E-30)}$$

* The commutator $[X, P_x]$ is an operator, and it should, actually, be written $[X, P_x] = i\hbar\mathbb{1}$. However, we shall often replace the identity operator $\mathbb{1}$ by the number 1, except when it is important to make the distinction.





where $R_1$, $R_2$, $R_3$, and $P_1$, $P_2$, $P_3$ designate respectively $X$, $Y$, $Z$ and $P_x$, $P_y$, $P_z$. Formulas (E-30) are called *canonical commutation relations.*

### b. R AND P ARE HERMITIAN

In order to show that $X$, for example, is a Hermitian operator, we can use formula (E-23):

$$\langle \varphi | X | \psi \rangle = \int d^3r \; \varphi^*(\mathbf{r}) \; x \; \psi(\mathbf{r})$$

$$= \left[ \int d^3r \; \psi^*(\mathbf{r}) \; x \; \varphi(\mathbf{r}) \right]^*$$

$$= \langle \psi | X | \varphi \rangle^* \qquad \text{(E-31)}$$

From §B-4-e, we know that equation (E-31) is characteristic of a Hermitian operator.

Similar proofs show that $Y$ and $Z$ are also Hermitian. For $P_x$, $P_y$ and $P_z$, the $\{ | \mathbf{p} \rangle \}$ representation can be used, and the calculations are then analogous to the preceding ones.

It is interesting to show that **P** is Hermitian by using equation (E-26), which gives its action in the $\{ | \mathbf{r} \rangle \}$ representation. Consider, for example, formula (E-27) and integrate it by parts:

$$\langle \varphi | P_x | \psi \rangle = \frac{\hbar}{i} \int dy \; dz \int_{-\infty}^{+\infty} dx \; \varphi^*(\mathbf{r}) \; \frac{\partial}{\partial x} \; \psi(\mathbf{r})$$

$$= \frac{\hbar}{i} \int dy \; dz \left\{ \left[ \varphi^*(\mathbf{r}) \; \psi(\mathbf{r}) \right]_{x=-\infty}^{x=+\infty} - \int_{-\infty}^{+\infty} dx \; \psi(\mathbf{r}) \; \frac{\partial}{\partial x} \varphi^*(\mathbf{r}) \right\} \qquad \text{(E-32)}$$

Since the integral which yields the scalar product $\langle \varphi | \psi \rangle$ is convergent, $\varphi^*(\mathbf{r})\psi(\mathbf{r})$ approaches zero when $x \longrightarrow \pm\infty$. The first term on the right hand side of (E-32) is therefore equal to zero, and:

$$\langle \varphi | P_x | \psi \rangle = -\frac{\hbar}{i} \int d^3r \; \psi(\mathbf{r}) \; \frac{\partial}{\partial x} \varphi^*(\mathbf{r})$$

$$= \left[ \frac{\hbar}{i} \int d^3r \; \psi^*(\mathbf{r}) \; \frac{\partial}{\partial x} \varphi(\mathbf{r}) \right]^*$$

$$= \langle \psi | P_x | \varphi \rangle^* \qquad \text{(E-33)}$$

It can be seen that the presence of the imaginary number $i$ is essential. The differential operator $\frac{\partial}{\partial x}$, acting on the functions of $\mathscr{F}$, is not Hermitian, because of the sign change which is introduced by the integration by parts. However, $i\frac{\partial}{\partial x}$ is Hermitian, as is $\frac{\hbar}{i}\frac{\partial}{\partial x}$.

### c. EIGENVECTORS OF R AND P

Consider the action of the $X$ operator on the ket $| \mathbf{r}_0 \rangle$; according to (E-22-a), we have:

$$\langle \mathbf{r} | X | \mathbf{r}_0 \rangle = x \langle \mathbf{r} | \mathbf{r}_0 \rangle = x \; \delta(\mathbf{r} - \mathbf{r}_0) = x_0 \; \delta(\mathbf{r} - \mathbf{r}_0) = x_0 \langle \mathbf{r} | \mathbf{r}_0 \rangle \qquad \text{(E-34)}$$

This equation expresses the fact that the components, in the $\{|\mathbf{r}\rangle\}$ representation, of the ket $X|\mathbf{r}_0\rangle$ are equal to those of the ket $|\mathbf{r}_0\rangle$ multiplied by $x_0$. We therefore have:

$$X|\mathbf{r}_0\rangle = x_0|\mathbf{r}_0\rangle \qquad \text{(E-35)}$$

An analogous argument shows that the kets $|\mathbf{r}_0\rangle$ are also eigenvectors of the $Y$ and $Z$ operators. Omitting the index zero which then becomes unnecessary, we can write:

$$\boxed{\begin{aligned} X|\mathbf{r}\rangle &= x|\mathbf{r}\rangle \\ Y|\mathbf{r}\rangle &= y|\mathbf{r}\rangle \\ Z|\mathbf{r}\rangle &= z|\mathbf{r}\rangle \end{aligned}} \qquad \text{(E-36)}$$

The kets $|\mathbf{r}\rangle$ are therefore the eigenkets common to $X$, $Y$ and $Z$. Thus the notation $|\mathbf{r}\rangle$ which we chose above is justified : each eigenvector is labelled by a vector $\mathbf{r}$, whose components $x$, $y$, $z$ represent three continuous indices which correspond to the eigenvalues of $X$, $Y$, $Z$.

Similar arguments can be elaborated for the $\mathbf{P}$ operator, placing ourselves, this time, in the $\{|\mathbf{p}\rangle\}$ representation. We then obtain:

$$\boxed{\begin{aligned} P_x|\mathbf{p}\rangle &= p_x|\mathbf{p}\rangle \\ P_y|\mathbf{p}\rangle &= p_y|\mathbf{p}\rangle \\ P_z|\mathbf{p}\rangle &= p_z|\mathbf{p}\rangle \end{aligned}} \qquad \text{(E-37)}$$

COMMENT:

This result can also be derived from equation (E-26), which gives the action of $\mathbf{P}$ in the $\{|\mathbf{r}\rangle\}$ representation. Using (E-9), we find:

$$\begin{aligned}\langle \mathbf{r}|P_x|\mathbf{p}\rangle &= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle \mathbf{r}|\mathbf{p}\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\,(2\pi\hbar)^{-3/2}\,e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} \\ &= p_x\,(2\pi\hbar)^{-3/2}\,e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} = p_x\langle \mathbf{r}|\mathbf{p}\rangle \end{aligned} \qquad \text{(E-38)}$$

All the components of the ket $P_x|\mathbf{p}\rangle$ in the $\{|\mathbf{r}\rangle\}$ representation can be obtained by multiplying those of $|\mathbf{p}\rangle$ by the constant $p_x$: $|\mathbf{p}\rangle$ is an eigenket of $P_x$ with the eigenvalue $p_x$.

### d. R AND P ARE OBSERVABLES

Relations (E-5-b) and (E-5-d) express the fact that the $\{|\mathbf{r}\rangle\}$ vectors and the $\{|\mathbf{p}\rangle\}$ vectors constitute bases in $\mathscr{E}_\mathbf{r}$. Therefore, $\mathbf{R}$ and $\mathbf{P}$ are observables.

Moreover, the specification of the three eigenvalues $x_0$, $y_0$, $z_0$ of $X$, $Y$, $Z$ uniquely determines the corresponding eigenvector $|\mathbf{r}_0\rangle$ : in the $\{|\mathbf{r}\rangle\}$ representation, its coordinates are $\delta(x - x_0)\delta(y - y_0)\delta(z - z_0)$. The set of the three operators $X$, $Y$, $Z$ therefore constitutes a C.S.C.O. in $\mathscr{E}_\mathbf{r}$.





It can be shown in the same way that the three components $P_x$, $P_y$, $P_z$ of $\mathbf{P}$ also constitute a C.S.C.O. in $\mathscr{E}_\mathbf{r}$.

Note that, in $\mathscr{E}_\mathbf{r}$, $X$ does not constitute a C.S.C.O. by itself. When the $x_0$ index is fixed, $y_0$ and $z_0$ can take on any real values. Thus, each eigenvalue $x_0$ is infinitely degenerate. On the other hand, in the state space $\mathscr{E}_x$ of a one-dimensional problem, $X$ constitutes a C.S.C.O. : the eigenvalue $x_0$ uniquely determines the corresponding eigenket $|x_0\rangle$, its coordinates being $\delta(x - x_0)$ in the $\{|x\rangle\}$ representation.

COMMENT:

We have found two C.S.C.O.'s in $\mathscr{E}_\mathbf{r}$, $\{X, Y, Z\}$ and $\{P_x, P_y, P_z\}$. We shall encounter others later. Consider, for example, the set $\{X, P_y, P_z\}$: these three observables commute (equations (E-30)); moreover, if the three eigenvalues $x_0$, $p_{0y}$ and $p_{0z}$ are fixed, there corresponds to them only one ket, whose associated wave function is written:

$$\psi_{x_0,p_{0y},p_{0z}}(x, y, z) = \delta(x - x_0)\,\frac{1}{2\pi\hbar}\,e^{\frac{i}{\hbar}(p_{0y}y + p_{0z}z)} \qquad \text{(E-39)}$$

# F. TENSOR PRODUCT OF STATE SPACES*

## 1. Introduction

We introduced the state space of a physical system using the concept of a one-particle wave function. However, our reasoning has involved sometimes one- and sometimes three-dimensional wave functions. Now it is clear that the space of square-integrable functions is not the same for functions of one variable $\psi(x)$ as for functions of three variables $\psi(\mathbf{r})$: $\mathscr{E}_\mathbf{r}$ and $\mathscr{E}_x$ are therefore different spaces. Nevertheless, $\mathscr{E}_\mathbf{r}$ appears to be essentially a generalization of $\mathscr{E}_x$. Does there exist a more precise relation between these two spaces?

In this section, we are going to define and study the operation of taking the tensor product of vector spaces**, and apply it to state spaces. This will answer, in particular, the question we have just asked : $\mathscr{E}_\mathbf{r}$ can be constructed from $\mathscr{E}_x$ and two other spaces, $\mathscr{E}_y$ and $\mathscr{E}_z$, which are isomorphic to it (§ F-4-a below).

In the same way, we shall be concerned later (chapters IV and IX) with the existence, for certain particles, of an intrinsic angular momentum or spin. In addition to the external degrees of freedom (position, momentum), which are treated using the observables $\mathbf{R}$ and $\mathbf{P}$ defined in $\mathscr{E}_\mathbf{r}$, it will be necessary to take into account the internal degrees of freedom and to introduce spin observables which act in a spin state space $\mathscr{E}_s$. The state space $\mathscr{E}$ of a particle with spin will then be seen to be the tensor product of $\mathscr{E}_\mathbf{r}$ and $\mathscr{E}_s$.

* This section is not necessary for the understanding of chapter III. One can study it later when it becomes necessary to use tensor products (complement $D_{IV}$, or chapter IX).

** This operation is sometimes called the "Kronecker product".