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This chapter is intended to be a general survey of the basic mathematical tools used in quantum mechanics. We shall give a simple condensed presentation aimed at facilitating the study of subsequent chapters for readers unfamiliar with these tools. We make no attempt to be mathematically complete and rigorous. We feel it preferable to limit ourselves to a practical point of view, uniting in a single chapter the various concepts which are useful in quantum mechanics. In particular, we wish to stress the convenience of the Dirac notation for carrying out the various calculations which we shall have to perform.

In this spirit, we shall try to simplify the discussion as much as possible. Neither the general definitions nor the rigorous proofs which would be required by a mathematician are to be found here. For example, we shall sometimes speak of infinite-dimensional spaces and reason as if they had a finite number of dimensions. Moreover, many terms (square-integrable functions, basis, etc...) will be employed with a meaning which, although commonly used in physics, is not exactly the one used in pure mathematics.

We begin in § A by studying the wave functions introduced in chapter I. We show that these wave functions belong to an abstract vector space, which we call the "wave function space $\mathscr{F}$". This study will be carried out in detail as it introduces some basic concepts of the mathematical formalism of quantum mechanics : scalar products, linear operators, basis, etc... Starting in § B, we shall develop a more general formalism, characterizing the state of a system by a "state vector" belonging to a vector space : the "state space $\mathscr{E}$". Dirac notation, which greatly simplifies calculations in this formalism, is introduced. § C is intended to study the idea of a representation. The reading of § D is particularly recommended to the reader who is unfamiliar with the diagonalization of an operator : this operation will be constantly useful to us in what follows. In § E, we treat two important examples of representations. In particular, we show how the wave functions studied in § A are the "components" of state vectors in a particular representation. Finally, we introduce in § F the concept of a tensor product. This concept will be illustrated more concretely by a simple example in complement D_{IV}.

A. ONE-PARTICLE WAVE FUNCTION SPACE

The probabilistic interpretation of the wave function $\psi(\mathbf{r}, t)$ of a particle was given in the preceding chapter : $|\psi(\mathbf{r}, t)|^2 d^3r$ represents the probability of finding, at time t, the particle in a volume $d^3r = dx\,dy\,dz$ about the point $\mathbf{r}$. The total probability of finding the particle somewhere in space is equal to 1, so we must have :

$$\int d^3r\, |\psi(\mathbf{r}, t)|^2 = 1 \tag{A-1}$$

where the integration extends over all space.

Thus, we are led to studying the set of square-integrable functions. These are functions for which the integral (A-1) converges. This set is called L^2 by mathematicians and it has the structure of a Hilbert space.

From a physical point of view, it is clear that the set L^2 is too wide in scope: given the meaning attributed to $|\psi(\mathbf{r}, t)|^2$, the wave functions which are actually

used possess certain properties of regularity. We can only retain the functions $\psi(\mathbf{r}, t)$ which are everywhere defined, continuous, and infinitely differentiable (for example, to state that a function is really discontinuous at a given point in space has no physical meaning, since no experiment enables us to have access to real phenomena on a very small scale, say of 10^{-30} m). It is also possible to confine ourselves to wave functions which have a bounded domain (which makes it certain that the particle can be found within a finite region of space, for example inside the laboratory). We shall not try to give a precise, general list of these supplementary conditions: we shall call $\mathscr{F}$ the set of wave functions composed of sufficiently regular functions of L^2 ($\mathscr{F}$ is a subspace of L^2).

1. Structure of the wave function space $\mathscr{F}$

a. $\mathscr{F}$ AS A VECTOR SPACE

It can easily be shown that $\mathscr{F}$ satisfies all the criteria of a vector space. As an example, we demonstrate that if $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r}) \in \mathscr{F}$, then* :

$$\psi(\mathbf{r}) = \lambda_1\psi_1(\mathbf{r}) + \lambda_2\psi_2(\mathbf{r}) \in \mathscr{F} \tag{A-2}$$

where λ_1 and λ_2 are two arbitrary complex numbers.

In order to show that $\psi(\mathbf{r})$ is square-integrable, expand $|\psi(\mathbf{r})|^2$:

$$|\psi(\mathbf{r})|^2 = |\lambda_1|^2\,|\psi_1(\mathbf{r})|^2 + |\lambda_2|^2\,|\psi_2(\mathbf{r})|^2 + \lambda_1^*\lambda_2\psi_1^*(\mathbf{r})\psi_2(\mathbf{r}) + \lambda_1\lambda_2^*\psi_1(\mathbf{r})\psi_2^*(\mathbf{r}) \tag{A-3}$$

The last two terms of (A-3) have the same modulus, which has as an upper limit:

$$|\lambda_1|\,|\lambda_2|\,[|\psi_1(\mathbf{r})|^2 + |\psi_2(\mathbf{r})|^2]$$

$|\psi(\mathbf{r})|^2$ is therefore smaller than a function whose integral converges, since ψ_1 and ψ_2 are square-integrable.

b. THE SCALAR PRODUCT

α. *Definition*

With each pair of elements of $\mathscr{F}$, $\varphi(\mathbf{r})$ and $\psi(\mathbf{r})$, taken in this order, we associate a *complex number*, denoted by (φ, ψ), which, by definition, is equal to:

$$\boxed{(\varphi, \psi) = \int d^3r\ \varphi^*(\mathbf{r})\ \psi(\mathbf{r})} \tag{A-4}$$

(φ, ψ) is the *scalar product of* $\psi(\mathbf{r})$ *by* $\varphi(\mathbf{r})$ [this integral always converges if φ and ψ belong to $\mathscr{F}$].

β. *Properties*

They follow from definition (A-4) :

* The symbol $\in$ signifies : "belongs to".

$$(\varphi, \psi) = (\psi, \varphi)^* \tag{A-5}$$

$$(\varphi, \lambda_1\psi_1 + \lambda_2\psi_2) = \lambda_1(\varphi, \psi_1) + \lambda_2(\varphi, \psi_2) \tag{A-6}$$

$$(\lambda_1\varphi_1 + \lambda_2\varphi_2, \psi) = \lambda_1^*(\varphi_1, \psi) + \lambda_2^*(\varphi_2, \psi) \tag{A-7}$$

The scalar product is *linear* with respect to the second function of the pair, *anti-linear* with respect to the first one. If $(\varphi, \psi) = 0$, $\varphi(\mathbf{r})$ and $\psi(\mathbf{r})$ are said to be *orthogonal.*

$$(\psi, \psi) = \int d^3r\, |\psi(\mathbf{r})|^2 \tag{A-8}$$

is a *real, positive* number, which is *zero if and only if* $\psi(\mathbf{r}) \equiv 0$.

$\sqrt{(\psi, \psi)}$ is called the norm of $\psi(\mathbf{r})$ [it can easily be verified that this number has all the properties of a norm]. The scalar product chosen above thus permits the definition of a norm in $\mathcal{F}$.

Let us mention, finally, (*cf.* complement A_{II}) the *Schwarz inequality*:

$$|(\psi_1, \psi_2)| \leqslant \sqrt{(\psi_1, \psi_1)}\ \sqrt{(\psi_2, \psi_2)} \tag{A-9}$$

This becomes an equality if and only if the two functions ψ_1 and ψ_2 are proportional.

c. LINEAR OPERATORS

α. *Definition*

A linear operator A is, by definition, a mathematical entity which associates with every function $\psi(\mathbf{r}) \in \mathcal{F}$ another function $\psi'(\mathbf{r})$, the correspondence being linear:

$$\psi'(\mathbf{r}) = A\psi(\mathbf{r}) \tag{A-10-a}$$

$$A[\lambda_1\psi_1(\mathbf{r}) + \lambda_2\psi_2(\mathbf{r})] = \lambda_1 A\psi_1(\mathbf{r}) + \lambda_2 A\psi_2(\mathbf{r}) \tag{A-10-b}$$

Let us cite some simple examples of linear operators: the parity operator Π, whose definition is:

$$\Pi\psi(x, y, z) = \psi(-x, -y, -z) \tag{A-11}$$

the operator which performs a multiplication by x, which we shall call X, and which is defined by:

$$X\psi(x, y, z) = x\psi(x, y, z) \tag{A-12}$$

finally, the operator which differentiates with respect to x, which we shall call D_x, and whose definition is:

$$D_x\psi(x, y, z) = \frac{\partial\psi(x, y, z)}{\partial x} \tag{A-13}$$

[the two operators X and D_x, acting on a function $\psi(\mathbf{r}) \in \mathcal{F}$, can transform it into a function which is no longer necessarily square-integrable].

β. *Product of operators*

Let A and B be two linear operators. Their product AB is defined by:

$$(AB)\psi(\mathbf{r}) = A[B\psi(\mathbf{r})] \tag{A-14}$$

B is first allowed to act on $\psi(\mathbf{r})$, which gives $\varphi(\mathbf{r}) = B\psi(\mathbf{r})$, then A operates on the new function $\varphi(\mathbf{r})$.

In general, $AB \neq BA$. We call the *commutator* of A and B the operator written $[A, B]$ and defined by

$$[A, B] = AB - BA \tag{A-15}$$

We shall calculate, as an example, the commutator $[X, D_x]$. In order to do this, we shall take an arbitrary function $\psi(\mathbf{r})$:

$$\begin{aligned}[X, D_x]\ \psi(\mathbf{r}) &= \left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)\psi(\mathbf{r}) \\ &= x\frac{\partial}{\partial x}\psi(\mathbf{r}) - \frac{\partial}{\partial x}[x\psi(\mathbf{r})] \\ &= x\frac{\partial}{\partial x}\psi(\mathbf{r}) - \psi(\mathbf{r}) - x\frac{\partial}{\partial x}\psi(\mathbf{r}) = -\psi(\mathbf{r})\end{aligned} \tag{A-16}$$

Since this is true for all $\psi(\mathbf{r})$, it can be deduced that:

$$[X, D_x] = -1 \tag{A-17}$$

2. Discrete orthonormal bases in $\mathcal{F}$: $\{ u_i(\mathbf{r}) \}$

a. DEFINITION

Consider a countable set of functions of $\mathcal{F}$, labeled by a discrete index i ($i = 1, 2, \ldots, n, \ldots$):

$$u_1(\mathbf{r}) \in \mathcal{F},\quad u_2(\mathbf{r}) \in \mathcal{F},\quad \ldots,\quad u_i(\mathbf{r}) \in \mathcal{F},\quad \ldots$$

– The set $\{u_i(\mathbf{r})\}$ is *orthonormal* if:

$$(u_i, u_j) = \int d^3r\ u_i^*(\mathbf{r})\ u_j(\mathbf{r}) = \delta_{ij} \tag{A-18}$$

where δ_{ij}, the Kronecker delta function, is equal to 1 for $i = j$ and to 0 for $i \neq j$.

– It constitutes a *basis** if every function $\psi(\mathbf{r}) \in \mathcal{F}$ can be expanded in one and only one way in terms of the $u_i(\mathbf{r})$:

$$\psi(\mathbf{r}) = \sum_i c_i\, u_i(\mathbf{r}) \tag{A-19}$$

* When the set $\{ u_i(\mathbf{r}) \}$ constitutes a basis, it is sometimes said to be a complete set of functions. It must be noted that the word complete is used with a meaning different from the one it usually has in mathematics.

b. COMPONENTS OF A WAVE FUNCTION IN THE $\{ u_i(\mathbf{r}) \}$ BASIS

Multiply the two sides of (A-19) by $u_j^*(\mathbf{r})$ and integrate over all space. From (A-6) and (A-18)* :

$$(u_j, \psi) = \left(u_j, \sum_i c_i u_i \right) = \sum_i c_i (u_j, u_i)$$

$$= \sum_i c_i \delta_{ij} = c_j \tag{A-20}$$

that is:

$$\boxed{c_i = (u_i, \psi) = \int d^3r \; u_i^*(\mathbf{r}) \; \psi(\mathbf{r})} \tag{A-21}$$

The component c_i of $\psi(\mathbf{r})$ on $u_i(\mathbf{r})$ is therefore equal to the scalar product of $\psi(\mathbf{r})$ by $u_i(\mathbf{r})$. Once the $\{ u_i(\mathbf{r}) \}$ basis has been chosen, it is equivalent to specify $\psi(\mathbf{r})$ or the set of its components c_i with respect to the basis functions. The set of numbers c_i is said to *represent* $\psi(\mathbf{r})$ in the $\{ u_i(\mathbf{r}) \}$ basis.

COMMENTS:

(*i*) Note the analogy with an orthonormal basis $\{ \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \}$ of the ordinary three-dimensional space, R^3. The fact that $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ are orthogonal and unitary can indeed be expressed by:

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \qquad (i, j = 1, 2, 3) \tag{A-22}$$

Any vector $\mathbf{V}$ of R^3 can be expanded in this basis:

$$\mathbf{V} = \sum_{i=1}^{3} v_i \; \mathbf{e}_i \tag{A-23}$$

with

$$v_i = \mathbf{e}_i \cdot \mathbf{V} \tag{A-24}$$

Formulas (A-18), (A-19) and (A-21) thus generalize, as it were, the well-known formulas, (A-22), (A-23) and (A-24). However, it must be noted that the v_i are real numbers, while the c_i are complex numbers.

(*ii*) The same function $\psi(\mathbf{r})$ obviously has different components in two different bases. We shall study the problem of a change in basis later.

(*iii*) We can also, in the $\{ u_i(\mathbf{r}) \}$ basis, represent a linear operator A by a set of numbers which can be arranged in the form of a matrix. We shall take up this question again in § C, after we have introduced Dirac notation.

c. EXPRESSION FOR THE SCALAR PRODUCT IN TERMS OF THE COMPONENTS

Let $\varphi(\mathbf{r})$ and $\psi(\mathbf{r})$ be two wave functions which can be expanded as follows:

$$\varphi(\mathbf{r}) = \sum_i b_i \, u_i(\mathbf{r})$$

$$\psi(\mathbf{r}) = \sum_j c_j \, u_j(\mathbf{r}) \tag{A-25}$$

* To be completely rigorous, one should make certain that one can interchange $\sum_i$ and $\int d^3r$. We shall systematically ignore this kind of problem.

Their scalar product can be calculated by using (A-6), (A-7) and (A-18):

$$(\varphi, \psi) = \left(\sum_i b_i u_i, \sum_j c_j u_j \right) = \sum_{i,j} b_i^* c_j \, (u_i, u_j)$$

$$= \sum_{i,j} b_i^* c_j \, \delta_{ij}$$

that is:

$$\boxed{(\varphi, \psi) = \sum_i b_i^* c_i} \tag{A-26}$$

In particular:

$$\boxed{(\psi, \psi) = \sum_i |c_i|^2} \tag{A-27}$$

The scalar product of two wave functions (or the square of the norm of a wave function) can thus be very simply expressed in terms of the components of these functions in the $\{ u_i(\mathbf{r}) \}$ basis.

COMMENT:

Let $\mathbf{V}$ and $\mathbf{W}$ be two vectors of R^3, with components v_i and w_j. The analytic expression of their scalar product is well-known:

$$\mathbf{V} \cdot \mathbf{W} = \sum_{i=1}^{3} v_i \, w_i \tag{A-28}$$

Formula (A-26) can therefore be considered to be a generalization of (A-28).

d. CLOSURE RELATION

Relation (A-18), called the orthonormalization relation, expresses the fact that the functions of the set $\{ u_i(\mathbf{r}) \}$ are normalized to 1 and orthogonal with respect to each other. We are now going to establish another relation, called the closure relation, which expresses the fact that this set constitutes a basis.

If $\{ u_i(\mathbf{r}) \}$ is a basis of $\mathscr{F}$, there exists an expansion such as (A-19) for every function $\psi(\mathbf{r}) \in \mathscr{F}$. Substitute into (A-19) expression (A-21) for the various components c_i [the name of the integration variable must be changed, since $\mathbf{r}$ already appears in (A-19)]:

$$\psi(\mathbf{r}) = \sum_i c_i \, u_i(\mathbf{r}) = \sum_i (u_i, \psi) \, u_i(\mathbf{r})$$

$$= \sum_i \left[\int d^3r' \; u_i^*(\mathbf{r}') \; \psi(\mathbf{r}') \right] u_i(\mathbf{r}) \tag{A-29}$$

Interchanging $\sum_i$ and $\int d^3r'$, we obtain:

$$\psi(\mathbf{r}) = \int d^3r' \; \psi(\mathbf{r}') \left[\sum_i u_i(\mathbf{r}) \; u_i^*(\mathbf{r}') \right] \tag{A-30}$$

$\sum_i u_i(\mathbf{r})u_i^*(\mathbf{r}')$is therefore a function $F(\mathbf{r}, \mathbf{r}')$ of $\mathbf{r}$ and of $\mathbf{r}'$ such that, for every function $\psi(\mathbf{r})$, we have:

$$\psi(\mathbf{r}) = \int d^3r' \ \psi(\mathbf{r}') \ F(\mathbf{r}, \mathbf{r}') \tag{A-31}$$

Equation (A-31) is characteristic of the function $\delta(\mathbf{r} - \mathbf{r}')$ (*cf.* appendix II). From this it can be deduced that:

$$\boxed{\sum_i u_i(\mathbf{r}) \ u_i^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')} \tag{A-32}$$

Reciprocally, if an orthonormal set $\{ u_i(\mathbf{r}) \}$ satisfies the closure relation (A-32), it constitutes a basis. Any function $\psi(\mathbf{r})$ can indeed be written in the form:

$$\psi(\mathbf{r}) = \int d^3r' \ \psi(\mathbf{r}') \ \delta(\mathbf{r} - \mathbf{r}') \tag{A-33}$$

Substituting expression (A-32) for $\delta(\mathbf{r} - \mathbf{r}')$ into this expression, we obtain formula (A-30). To return to (A-29), all we must do is again interchange summation and integration. This equation then expresses the fact that $\psi(\mathbf{r})$ can always be expanded in terms of the $u_i(\mathbf{r})$ and gives the coefficients of this expansion.

COMMENT:

We shall re-examine the closure relation using the Dirac notation in § C, and we shall see that it can be given a simple geometric interpretation.

3. Introduction of "bases" not belonging to $\mathscr{F}$

The $\{ u_i(\mathbf{r}) \}$ bases studied above are composed of square-integrable functions. It can also be convenient to introduce "bases" of functions not belonging to either $\mathscr{F}$ or L^2, but in terms of which any wave function $\psi(\mathbf{r})$ can nevertheless be expanded. We are going to give examples of such bases and we shall show how it is possible to extend to them the important formulas which were established in the preceding section.

a. PLANE WAVES

For simplicity, we treat the one-dimensional case. We shall therefore study square-integrable functions $\psi(x)$ which depend only on the x variable. In chapter I we saw the advantage of using the Fourier transform $\bar{\psi}(p)$ of $\psi(x)$:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \mathrm{d}p \ \bar{\psi}(p) \, \mathrm{e}^{ipx/\hbar} \tag{A-34-a}$$

$$\bar{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \mathrm{d}x \ \psi(x) \, \mathrm{e}^{-ipx/\hbar} \tag{A-34-b}$$

Consider the function $v_p(x)$, defined by:

$$\boxed{v_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{ipx/\hbar}} \tag{A-35}$$

$v_p(x)$ is a plane wave, with the wave vector $p/\hbar$. The integral over the whole x axis of $|v_p(x)|^2 = \frac{1}{2\pi\hbar}$ diverges. Therefore $v_p(x) \notin \mathscr{F}_x$. We shall designate by $\{ v_p(x) \}$ the set of all plane waves, that is, of all functions $v_p(x)$ corresponding to the various values of p. The number p, which varies continuously between $-\infty$ and $+\infty$, will be considered as a *continuous index* which permits us to label the various functions of the set $\{ v_p(x) \}$ [recall that the index i used for the set $\{ u_i(\mathbf{r}) \}$ considered above was *discrete*].

Formulas (A-34) can be rewritten using (A-35):

$$\boxed{\psi(x) = \int_{-\infty}^{+\infty} \mathrm{d}p \ \bar{\psi}(p) \ v_p(x)} \tag{A-36}$$

$$\boxed{\bar{\psi}(p) = (v_p, \psi) = \int_{-\infty}^{+\infty} \mathrm{d}x \ v_p^*(x) \ \psi(x)} \tag{A-37}$$

These two formulas can be compared to (A-19) and (A-21). Relation (A-36) expresses the idea that every function $\psi(x) \in \mathscr{F}_x$ can be expanded in one and only way in terms of the $v_p(x)$, that is, the plane waves. Since the index p varies continuously and not discretely, the summation $\sum_i$ appearing in (A-19) must be replaced by an integration over p. Relation (A-37), like (A-21), gives the component $\bar{\psi}(p)$ of $\psi(x)$ on $v_p(x)$ in the form of a scalar product* (v_p, ψ). The set of these components, which correspond to the various possible values of p, constitutes a function of p, $\bar{\psi}(p)$, the Fourier transform of $\psi(x)$.

Thus, $\bar{\psi}(p)$ is the analogue of c_i. These two complex numbers, which depend either on p or on i, represent the *components of the same function $\psi(x)$ in two different bases: $\{ v_p(x) \}$ and $\{ u_i(x) \}$.*

This point also appears clearly if we calculate the square of the norm of $\psi(x)$. According to Parseval's relation [app. I, formula (45)], we have:

$$\boxed{(\psi, \psi) = \int_{-\infty}^{+\infty} \mathrm{d}p \, |\bar{\psi}(p)|^2} \tag{A-38}$$

a formula which resembles (A-27), if we replace c_i by $\bar{\psi}(p)$ and $\sum_i$ by $\int \mathrm{d}p$.

Let us show that the $v_p(x)$ satisfy a closure relation. Using the formula [*cf.* appendix II, equation (34)]:

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}k \, \mathrm{e}^{iku} = \delta(u) \tag{A-39}$$

* We have only defined the scalar product for two square-integrable functions, but this definition can easily be extended to cases like this one, provided that the corresponding integral converges.

we find:

$$\boxed{\int_{-\infty}^{+\infty} dp\ v_p(x)\ v_p^*(x') = \frac{1}{2\pi}\int \frac{dp}{\hbar}\, e^{i\frac{p}{\hbar}(x-x')} = \delta(x - x')} \tag{A-40}$$

This formula is the analogue of (A-32) with, again, the substitution of $\int dp$ for $\sum_i$.

Finally, let us calculate the scalar product $(v_p, v_{p'})$ in order to see if there exists an equivalent of the orthonormalization relation. Again using (A-39), we obtain:

$$(v_p, v_{p'}) = \int_{-\infty}^{+\infty} dx\ v_p^*(x)\ v_{p'}(x)$$

that is:

$$\boxed{(v_p, v_{p'}) = \frac{1}{2\pi}\int \frac{dx}{\hbar}\, e^{i\frac{x}{\hbar}(p'-p)} = \delta(p - p')} \tag{A-41}$$

Compare (A-41) and (A-18). Instead of having two discrete indices i and j and a Kronecker delta δ_{ij}, we now have two continuous indices p and p' and a delta function of the difference between the indices, $\delta(p - p')$. Note that if we set $p = p'$, the scalar product (v_p, v_p) diverges; again we see that $v_p(x) \notin \mathscr{F}_x$. Although this constitutes a misuse of the term, we shall call (A-41) an "orthonormalization" relation. It is also sometimes said that the $v_p(x)$ are "orthonormalized in the Dirac sense".

The generalization to three dimensions presents no difficulties. We consider the plane waves:

$$v_{\mathbf{p}}(\mathbf{r}) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \tag{A-42}$$

The functions of the $\{ v_{\mathbf{p}}(\mathbf{r}) \}$ basis now depend on the three continuous indices p_x, p_y, p_z, condensed into the notation $\mathbf{p}$. It is then easy to show that the following formulas are valid:

$$\psi(\mathbf{r}) = \int d^3p\ \bar{\psi}(\mathbf{p})\ v_{\mathbf{p}}(\mathbf{r}) \tag{A-43}$$

$$\bar{\psi}(\mathbf{p}) = (v_{\mathbf{p}}, \psi) = \int d^3r\ v_{\mathbf{p}}^*(\mathbf{r})\ \psi(\mathbf{r}) \tag{A-44}$$

$$(\varphi, \psi) = \int d^3p\ \bar{\varphi}^*(\mathbf{p})\ \bar{\psi}(\mathbf{p}) \tag{A-45}$$

$$\int d^3p\ v_{\mathbf{p}}(\mathbf{r})\ v_{\mathbf{p}}^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \tag{A-46}$$

$$(v_{\mathbf{p}}, v_{\mathbf{p}'}) = \delta(\mathbf{p} - \mathbf{p}') \tag{A-47}$$

They represent the generalizations of (A-36), (A-37), (A-38), (A-40) and (A-41).

Thus the $v_{\mathbf{p}}(\mathbf{r})$ can be considered to constitute a "continuous basis". All the formulas established above for the discrete basis $\{ u_i(\mathbf{r}) \}$ can be extended to this continuous basis, using the correspondence rules summarized in table (II-1).

i	$\mathbf{p}$
$\sum_i$	$\int d^3p$
δ_{ij}	$\delta(\mathbf{p} - \mathbf{p}')$

Table (II-1)

b. "DELTA FUNCTIONS"

In the same way, let us introduce a set of functions of $\mathbf{r}$, $\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$, labeled by the continuous index $\mathbf{r}_0$ (condensed notation for x_0, y_0, z_0) and defined by:

$$\boxed{\xi_{\mathbf{r}_0}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_0)} \tag{A-48}$$

$\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$ represents the set of delta functions centered at the various points $\mathbf{r}_0$ of space; $\xi_{\mathbf{r}_0}(\mathbf{r})$ is obviously not square-integrable : $\xi_{\mathbf{r}_0}(\mathbf{r}) \notin \mathscr{F}$.

Then consider the following relations, which are valid for every function $\psi(\mathbf{r})$ belonging to $\mathscr{F}$:

$$\psi(\mathbf{r}) = \int d^3r_0\ \psi(\mathbf{r}_0)\ \delta(\mathbf{r} - \mathbf{r}_0) \tag{A-49}$$

$$\psi(\mathbf{r}_0) = \int d^3r\ \delta(\mathbf{r}_0 - \mathbf{r})\ \psi(\mathbf{r}) \tag{A-50}$$

They can be rewritten, using (A-48), in the form:

$$\boxed{\psi(\mathbf{r}) = \int d^3r_0\ \psi(\mathbf{r}_0)\ \xi_{\mathbf{r}_0}(\mathbf{r})} \tag{A-51}$$

$$\boxed{\psi(\mathbf{r}_0) = (\xi_{\mathbf{r}_0}, \psi) = \int d^3r\ \xi_{\mathbf{r}_0}^*(\mathbf{r})\ \psi(\mathbf{r})} \tag{A-52}$$

(A-51) expresses the fact that every function $\psi(\mathbf{r}) \in \mathscr{F}$ can be expanded in one and only one way in terms of the $\xi_{\mathbf{r}_0}(\mathbf{r})$. (A-52) shows that the component of $\psi(\mathbf{r})$ on the function $\xi_{\mathbf{r}_0}(\mathbf{r})$ (we are dealing here with real basis functions) is precisely the value $\psi(\mathbf{r}_0)$ of $\psi(\mathbf{r})$ at the point $\mathbf{r}_0$. (A-51) and (A-52) are analogous to (A-19) and (A-21): we simply replace the discrete index i by the continuous index $\mathbf{r}_0$, and $\sum_i$ by $\int d^3r_0$.

$\psi(\mathbf{r}_0)$ is therefore the equivalent of c_i: these two complex numbers, which depend either on $\mathbf{r}_0$ or on i, represent the components of the same function $\psi(\mathbf{r})$ in two different bases: $\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$ and $\{ u_i(\mathbf{r}) \}$.

Formula (A-26) becomes here:

$$\boxed{(\varphi, \psi) = \int d^3r_0 \ \varphi^*(\mathbf{r}_0)\ \psi(\mathbf{r}_0)} \tag{A-53}$$

We see that the application of (A-26) to the case of the continuous basis $\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$ results in the definition (A-4) of the scalar product.

Finally, note that the $\xi_{\mathbf{r}_0}(\mathbf{r})$ satisfy " orthonormalization " and closure relations of the same type as those for the $v_{\mathbf{p}}(\mathbf{r})$. Thus we have [formula (28) of appendix II]:

$$\boxed{\int d^3r_0 \ \xi_{\mathbf{r}_0}(\mathbf{r})\ \xi^*_{\mathbf{r}_0}(\mathbf{r}') = \int d^3r_0 \ \delta(\mathbf{r} - \mathbf{r}_0)\ \delta(\mathbf{r}' - \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}')} \tag{A-54}$$

and:

$$\boxed{(\xi_{\mathbf{r}_0}, \xi_{\mathbf{r}'_0}) = \int d^3r \ \delta(\mathbf{r} - \mathbf{r}_0)\ \delta(\mathbf{r} - \mathbf{r}'_0) = \delta(\mathbf{r}_0 - \mathbf{r}'_0)} \tag{A-55}$$

All the formulas established for the discrete basis $\{ u_i(\mathbf{r}) \}$ can thus be generalized for the continuous basis $\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$, using the correspondence rules summarized in table (II-2).

i	$\mathbf{r}_0$
$\sum_i$	$\int d^3r_0$
δ_{ij}	$\delta(\mathbf{r}_0 - \mathbf{r}'_0)$

Table (II-2)

IMPORTANT COMMENT:

The usefulness of the continuous bases which we have just introduced is revealed more clearly in what follows. However, we must not lose sight of the following point: *a physical state must always correspond to a square-integrable wave function.* In no case can $v_{\mathbf{p}}(\mathbf{r})$ or $\xi_{\mathbf{r}_0}(\mathbf{r})$ represent the state of a particle. These functions are nothing more than intermediaries, very useful in calculations involving operations on the wave functions $\psi(\mathbf{r})$ which are used to describe a physical state.

An analogous situation is encountered in classical optics, where the plane monochromatic wave is a mathematically very useful, but physically unrealizable, idealization. Even the most selective filters always permit the passage of a frequency band $\Delta\nu$, which may be very small but is never exactly zero.

The same holds true for the functions $\xi_{\mathbf{r}_0}(\mathbf{r})$. We can imagine a square-integrable wave function, localized about $\mathbf{r}_0$, for example:

$$\xi^{(\varepsilon)}_{\mathbf{r}_0}(\mathbf{r}) = \delta^{(\varepsilon)}(\mathbf{r} - \mathbf{r}_0) = \delta^{(\varepsilon)}(x - x_0)\delta^{(\varepsilon)}(y - y_0)\delta^{(\varepsilon)}(z - z_0)$$

where the $\delta^{(\varepsilon)}$ are functions which have a peak of width ε and amplitude $\frac{1}{\varepsilon}$, centered at x_0, y_0 or z_0, such that $\int_{-\infty}^{+\infty} \delta^{(\varepsilon)}(x - x_0)\, dx = 1$ (see § 1-b of appendix II for examples of such functions). When $\varepsilon \longrightarrow 0$, $\xi^{(\varepsilon)}_{\mathbf{r}_0}(\mathbf{r}) \longrightarrow \xi_{\mathbf{r}_0}(\mathbf{r})$, which is no longer square-integrable. But, in fact, it is impossible to have a physical state which corresponds to this limit: as localized as the physical state of a particle may be, ε is never exactly zero.

c. GENERALIZATION: CONTINUOUS "ORTHONORMAL" BASES

α. *Definition*

Generalizing the results obtained in the two preceding paragraphs, we shall call a *continuous "orthonormal" basis*, a set of functions of $\mathbf{r}$, $\{ w_\alpha(\mathbf{r}) \}$, labeled by a continuous index α, which satisfy the two following relations, called *orthonormalization* and *closure* relations:

$$\boxed{(w_\alpha, w_{\alpha'}) = \int d^3r \ w^*_\alpha(\mathbf{r})\ w_{\alpha'}(\mathbf{r}) = \delta(\alpha - \alpha')} \tag{A-56}$$

$$\boxed{\int d\alpha \ w_\alpha(\mathbf{r})\ w^*_\alpha(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')} \tag{A-57}$$

COMMENTS:

(*i*) If $\alpha = \alpha'$, (w_α, w_α) diverges. Therefore, $w_\alpha(\mathbf{r}) \notin \mathscr{F}$.

(*ii*) α can represent several indices, as is the case for $\mathbf{r}_0$ and $\mathbf{p}$ in the above examples.

(*iii*) It is possible to imagine a basis which includes both functions $u_i(\mathbf{r})$, labeled by a discrete index, and functions $w_\alpha(\mathbf{r})$, labeled by a continuous index. In this case, the set of $u_i(\mathbf{r})$ does not form a basis; the set of $w_\alpha(\mathbf{r})$ must be added to it.

Let us cite an example of this situation. Consider the case of the square well studied in § D-2-c of chapter I (see also complement H_1). As we shall see later, the set of stationary states of a particle in a time-independent potential constitutes a basis. For $E < 0$, we have discrete energy levels, to which correspond square-integrable wave functions labeled by a discrete index. But these are not the only possible stationary states. Equation (D-17) of chapter I is also satisfied, for all $E > 0$, by solutions which are bounded but which extend over all space and are thus not square-integrable.

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

$$\begin{aligned} &(u_i, u_j) = \delta_{ij} \\ &(w_\alpha, w_{\alpha'}) = \delta(\alpha - \alpha') \\ &(u_i, w_\alpha) = 0 \end{aligned} \tag{A-58}$$

And the closure relation becomes:

$$\sum_i u_i(\mathbf{r})\ u_i^*(\mathbf{r}') + \int d\alpha \ w_\alpha(\mathbf{r})\ w^*_\alpha(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \tag{A-59}$$

β. *Components of a wave function* $\psi(\mathbf{r})$

We can always write :

$$\psi(\mathbf{r}) = \int d^3r' \ \psi(\mathbf{r}') \ \delta(\mathbf{r} - \mathbf{r}') \tag{A-60}$$

Using the expression for $\delta(\mathbf{r} - \mathbf{r}')$ given by (A-57), and assuming that we can reverse the order of $\int d^3r'$ and $\int d\alpha$, we obtain :

$$\psi(\mathbf{r}) = \int d\alpha \left[\int d^3r' \ w_\alpha^*(\mathbf{r}') \ \psi(\mathbf{r}') \right] w_\alpha(\mathbf{r})$$

that is : $\boxed{\psi(\mathbf{r}) = \int d\alpha \ c(\alpha) \ w_\alpha(\mathbf{r})}$ (A-61)

with $\boxed{c(\alpha) = (w_\alpha, \psi) = \int d^3r' \ w_\alpha^*(\mathbf{r}') \ \psi(\mathbf{r}')}$ (A-62)

(A-61) expresses the fact that every wave function $\psi(\mathbf{r})$ has a unique expansion in terms of the $w_\alpha(\mathbf{r})$. The component $c(\alpha)$ of $\psi(\mathbf{r})$ on $w_\alpha(\mathbf{r})$ is equal, according to (A-62), to the scalar product (w_α, ψ).

γ. *Expression for the scalar product and the norm in terms of the components*

Let $\varphi(\mathbf{r})$ and $\psi(\mathbf{r})$ be two square-integrable functions whose components in terms of the $w_\alpha(\mathbf{r})$ are known:

$$\varphi(\mathbf{r}) = \int d\alpha \ b(\alpha) \ w_\alpha(\mathbf{r}) \tag{A-63}$$

$$\psi(\mathbf{r}) = \int d\alpha' \ c(\alpha') \ w_{\alpha'}(\mathbf{r}) \tag{A-64}$$

Calculate their scalar product:

$$(\varphi, \psi) = \int d^3r \ \varphi^*(\mathbf{r}) \ \psi(\mathbf{r})$$

$$= \int d\alpha \int d\alpha' \ b^*(\alpha) \ c(\alpha') \int d^3r \ w_\alpha^*(\mathbf{r}) \ w_{\alpha'}(\mathbf{r}) \tag{A-65}$$

The last integral is given by (A-56):

$$(\varphi, \psi) = \int d\alpha \int d\alpha' \ b^*(\alpha) \ c(\alpha') \ \delta(\alpha - \alpha')$$

that is :

$$\boxed{(\varphi, \psi) = \int d\alpha \ b^*(\alpha) \ c(\alpha)} \tag{A-66}$$

In particular :

$$\boxed{(\psi, \psi) = \int d\alpha \ |c(\alpha)|^2} \tag{A-67}$$

All the formulas of § A-2 can thus be generalized, using the correspondence rules of table (II-3).

$i \longleftrightarrow \alpha$
$\sum_i \longleftrightarrow \int d\alpha$
$\delta_{ij} \longleftrightarrow \delta(\alpha - \alpha')$

Table (II-3)

The most important formulas established in this section are assembled in table (II-4). In fact, it is not necessary to remember them in this form : we shall see that the introduction of Dirac notation enables us to rederive them very simply.

Table (II-4)

	Discrete basis $\{ u_i(\mathbf{r}) \}$	Continuous basis $\{ w_\alpha(\mathbf{r}) \}$
Ortho-normalization relation	$(u_i, u_j) = \delta_{ij}$	$(w_\alpha, w_{\alpha'}) = \delta(\alpha - \alpha')$
Closure relation (the set constitutes a basis)	$\sum_i u_i(\mathbf{r}) \ u_i^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$	$\int d\alpha \ w_\alpha(\mathbf{r}) \ w_\alpha^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$
Expansion of a wave function $\psi(\mathbf{r})$	$\psi(\mathbf{r}) = \sum_i c_i \ u_i(\mathbf{r})$	$\psi(\mathbf{r}) = \int d\alpha \ c(\alpha) \ w_\alpha(\mathbf{r})$
Expression for the components of $\psi(\mathbf{r})$	$c_i = (u_i, \psi) = \int d^3r \ u_i^*(\mathbf{r}) \ \psi(\mathbf{r})$	$c(\alpha) = (w_\alpha, \psi) = \int d^3r \ w_\alpha^*(\mathbf{r}) \ \psi(\mathbf{r})$
Scalar product	$(\varphi, \psi) = \sum_i b_i^* c_i$	$(\varphi, \psi) = \int d\alpha \ b^*(\alpha) \ c(\alpha)$
Square of the norm	$(\psi, \psi) = \sum_i \lvert c_i \rvert^2$	$(\psi, \psi) = \int d\alpha \ \lvert c(\alpha) \rvert^2$

B. STATE SPACE. DIRAC NOTATION

1. Introduction

In chapter I, we stated the following postulate: the quantum state of a particle is defined, at a given instant, by a wave function $\psi(\mathbf{r})$. The probabilistic interpretation of this wave function requires that it be square-integrable. This requirement led us to study the $\mathscr{F}$-space (§ A). We then found, in particular, that the same function $\psi(\mathbf{r})$ can be represented by several distinct sets of components, each one corresponding to the choice of a basis [table (II-5)]. This result can be interpreted in the following manner: $\{ c_i \}$, or $\overline{\psi}(\mathbf{p})$, or $c(\alpha)$, characterizes the state of a particle just as well as the wave function $\psi(\mathbf{r})$ [if the basis being used has been specified previously]. Furthermore, $\psi(\mathbf{r})$ itself appears, in table (II-5), on the same footing as $\{ c_i \}$, $\overline{\psi}(\mathbf{p})$ and $c(\alpha)$: the value $\psi(\mathbf{r}_0)$ which the wave function takes on at a point $\mathbf{r}_0$ of space can be considered as its component with respect to a specific function $\xi_{\mathbf{r}_0}(\mathbf{r})$ of a particular basis (the δ function basis).

Basis	*Components of* $\psi(\mathbf{r})$
$u_i(\mathbf{r})$	c_i, $i = 1, 2, \ldots, n, \ldots$
$v_{\mathbf{p}}(\mathbf{r})$	$\overline{\psi}(\mathbf{p})$
$\xi_{\mathbf{r}_0}(\mathbf{r})$	$\psi(\mathbf{r}_0)$
$w_\alpha(\mathbf{r})$	$c(\alpha)$

Table (II-5)

We thus find ourselves in a situation which is analogous to the one encountered in ordinary space, R^3: the position of a point in space can be described by a set of three numbers, which are its coordinates with respect to a system of axes defined in advance. If one changes axes, another set of coordinates corresponds to the same point. But the geometrical vector concept and vector calculation enable us to avoid referring to a system of axes; this considerably simplifies both formulas and reasoning.

We are going to use a similar approach here: each quantum state of a particle will be characterized by a *state vector*, belonging to an abstract space, $\mathscr{E}_{\mathbf{r}}$, called the *state space* of a particle. The fact that the space $\mathscr{F}$ is a subspace of L^2 means that $\mathscr{E}_{\mathbf{r}}$ is a subspace of a Hilbert space. We are going to define the notation and the rules of vector calculation in $\mathscr{E}_{\mathbf{r}}$.

Actually, the introduction of state vectors and the state space does more than merely simplify the formalism. It also permits a generalization of the formalism. Indeed, there exist physical systems whose quantum description cannot be given by a wave function: we shall see in chapters IV and IX that this is the case when the spin degrees of freedom are taken into account, even for a single particle. Consequently, the first postulate that we shall set forth in

chapter III will be the following: *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.*

Therefore, in the rest of this chapter, we are going to develop a vector calculus in $\mathscr{E}$. The concepts which we are going to introduce and the results which we shall obtain are valid for whatever physical system we might consider. Nevertheless, to illustrate these concepts and results, we shall apply them to the simple case of a (spinless) particle, since this is the case we have previously considered.

We shall begin, in this paragraph, by defining the *Dirac notation*, which will prove to be very useful in the formal manipulations which we shall have to perform.

2. "Ket" vectors and "bra" vectors

a. ELEMENTS OF $\mathscr{E}$: KETS

α. *Notation*

Any element, or vector, of $\mathscr{E}$-space is called a *ket vector*, or, more simply, a *ket*. It is represented by the symbol $|\ \rangle$, inside which is placed a distinctive sign which enables us to distinguish the corresponding ket from all others, for example: $|\ \psi\ \rangle$.

In particular, since the concept of a wave function is now familiar to us, we shall define the space $\mathscr{E}_{\mathbf{r}}$ of the states of a particle by associating with every square-integrable function $\psi(\mathbf{r})$ a ket vector $|\ \psi\ \rangle$ of $\mathscr{E}_{\mathbf{r}}$:

$$\psi(\mathbf{r}) \in \mathscr{F} \iff |\ \psi\ \rangle \in \mathscr{E}_{\mathbf{r}} \tag{B-1}$$

Afterwards, we shall transpose the different operations which we introduced for $\mathscr{F}$ into $\mathscr{E}_{\mathbf{r}}$. Although $\mathscr{F}$ and $\mathscr{E}_{\mathbf{r}}$ are isomorphic, we shall carefully distinguish between them in order to avoid confusion and to reserve the possibilities of generalization mentioned above in § B-1. We stress the fact that an $\mathbf{r}$-dependence no longer appears in $|\ \psi\ \rangle$; only the letter ψ appears to remind us with which function it is associated. $\psi(\mathbf{r})$ will be interpreted (§ E) as the set of the components of the ket $|\ \psi\ \rangle$ in a particular basis, $\mathbf{r}$ playing the role of an index [*cf.* § A-3-b and table (II-5)]. Consequently, the procedure which we are adopting here consists in initially characterizing a vector by its components in a privileged coordinate system, which will later be treated on the same footing as all other coordinate systems.

We shall designate by $\mathscr{E}_x$ the state space of a (spinless) particle in only one dimension, that is, the abstract space constructed as in (B-1), but using wave functions which depend only on the x variable.

β. *Scalar product*

With each pair of kets $|\ \varphi\ \rangle$ and $|\ \psi\ \rangle$, taken in this order, we associate a complex number, which is their scalar product, $(|\ \varphi\ \rangle, |\ \psi\ \rangle)$, and which satisfies the various properties described by equations (A-5), (A-6) and (A-7). We shall

later rewrite these formulas in Dirac notation after we have introduced the concept of a "bra".

In $\mathscr{E}_r$, the scalar product of two kets will coincide with the scalar product defined above for the associated wave functions.

b. ELEMENTS OF THE DUAL SPACE $\mathscr{E}^*$ OF $\mathscr{E}$: BRAS

α. *Definition of the dual space $\mathscr{E}^*$*

Recall, first of all, the definition of a *linear functional* defined on the kets $|\psi\rangle$ of $\mathscr{E}$. A linear functional χ is a linear operation which associates a complex number with every ket $|\psi\rangle$:

$$|\psi\rangle \in \mathscr{E} \xrightarrow{\chi} \text{number } \chi(|\psi\rangle)$$
$$\chi(\lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle) = \lambda_1 \chi(|\psi_1\rangle) + \lambda_2 \chi(|\psi_2\rangle) \qquad \text{(B-2)}$$

Linear functional and linear operator must not be confused. In both cases, one is dealing with linear operations, but the former associates each ket with a complex number, while the latter associates another ket.

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

β. *Bra notation for the vectors of $\mathscr{E}^*$*

Any element, or vector, of the space $\mathscr{E}^*$ is called a *bra vector*, or, more simply, a *bra*. It is symbolized by $\langle\ |$. For example, the bra $\langle \chi |$ designates the linear functional χ and we shall henceforth use the notation $\langle \chi | \psi \rangle$ to denote the *number* obtained by causing the linear functional $\langle \chi | \in \mathscr{E}^*$ to act on the ket $|\psi\rangle \in \mathscr{E}$:

$$\boxed{\chi(|\psi\rangle) = \langle \chi | \psi \rangle} \qquad \text{(B-3)}$$

The origin of this terminology is the word "bracket", used to denote the symbol $\langle | \rangle$. Hence the name "bra" for the left-hand side, and the name "ket" for the right-hand side of this symbol.

c. CORRESPONDENCE BETWEEN KETS AND BRAS

α. *To every ket corresponds a bra*

The existence of a scalar product in $\mathscr{E}$ will now enable us to show that we can associate, with every ket $|\varphi\rangle \in \mathscr{E}$, an element of $\mathscr{E}^*$, that is, a bra, which will be denoted by $\langle \varphi |$.

The ket $|\varphi\rangle$ does indeed enable us to define a linear functional: the one which associates (in a linear way), with each ket $|\psi\rangle \in \mathscr{E}$, a complex number which is equal to the scalar product $(|\varphi\rangle, |\psi\rangle)$ of $|\psi\rangle$ by $|\varphi\rangle$. Let $\langle \varphi |$ be this linear functional; it is thus defined by the relation:

$$\boxed{\langle \varphi | \psi \rangle = (|\varphi\rangle, |\psi\rangle)} \qquad \text{(B-4)}$$

β. *This correspondance is antilinear*

In the space $\mathscr{E}$, the scalar product is antilinear with respect to the first vector. In the notation of (B-4), this is expressed by:

$$\begin{aligned}(\lambda_1 |\varphi_1\rangle + \lambda_2 |\varphi_2\rangle, |\psi\rangle) &= \lambda_1^*(|\varphi_1\rangle, |\psi\rangle) + \lambda_2^*(|\varphi_2\rangle, |\psi\rangle) \\ &= \lambda_1^* \langle \varphi_1 | \psi \rangle + \lambda_2^* \langle \varphi_2 | \psi \rangle \\ &= (\lambda_1^* \langle \varphi_1 | + \lambda_2^* \langle \varphi_2 |) |\psi\rangle \end{aligned} \qquad \text{(B-5)}$$

It appears from (B-5) that the bra associated with the ket $\lambda_1 |\varphi_1\rangle + \lambda_2 |\varphi_2\rangle$ is the bra $\lambda_1^* \langle \varphi_1 | + \lambda_2^* \langle \varphi_2 |$:

$$\boxed{\lambda_1 |\varphi_1\rangle + \lambda_2 |\varphi_2\rangle \Longrightarrow \lambda_1^* \langle \varphi_1 | + \lambda_2^* \langle \varphi_2 |} \qquad \text{(B-6)}$$

The ket $\Longrightarrow$ bra correspondence is therefore antilinear.

COMMENT:

If λ is a complex number, and $|\psi\rangle$ a ket, $\lambda |\psi\rangle$ is a ket ($\mathscr{E}$ is a vector space). We are sometimes led to write it as $|\lambda\psi\rangle$:

$$|\lambda\psi\rangle = \lambda |\psi\rangle \qquad \text{(B-7)}$$

One must then be careful to remember that $\langle \lambda\psi |$ *represents the bra* associated with the ket $|\lambda\psi\rangle$. Since the correspondence between a bra and a ket is antilinear, we have:

$$\langle \lambda\psi | = \lambda^* \langle \psi | \qquad \text{(B-8)}$$

γ. *Dirac notation for the scalar product*

We now have at our disposal two distinct notations for designating the scalar product of $|\psi\rangle$ by $|\varphi\rangle$: $(|\varphi\rangle, |\psi\rangle)$ or $\langle \varphi | \psi \rangle$, $\langle \varphi |$ being the bra associated with the ket $|\varphi\rangle$. Henceforth we shall use only the (Dirac) notation: $\langle \varphi | \psi \rangle$. Table (II-6) summarizes, in Dirac notation, the properties of the scalar product, already given in § A-1-b.

$$\boxed{\begin{aligned} &\langle \varphi | \psi \rangle = \langle \psi | \varphi \rangle^* && \text{(B-9)} \\ &\langle \varphi | \lambda_1\psi_1 + \lambda_2\psi_2 \rangle = \lambda_1 \langle \varphi | \psi_1 \rangle + \lambda_2 \langle \varphi | \psi_2 \rangle && \text{(B-10)} \\ &\langle \lambda_1\varphi_1 + \lambda_2\varphi_2 | \psi \rangle = \lambda_1^* \langle \varphi_1 | \psi \rangle + \lambda_2^* \langle \varphi_2 | \psi \rangle && \text{(B-11)} \\ &\langle \psi | \psi \rangle \text{ real, positive; zero if and only if } |\psi\rangle = 0 && \text{(B-12)} \end{aligned}}$$

δ. *Is there a ket to correspond to every bra?*

Although to every ket there corresponds a bra, we shall see in two examples chosen in $\mathscr{F}$, that it is possible to find bras which have no corresponding kets. We shall later show why this difficulty does not hinder us in quantum mechanics.

(*i*) Counter-examples chosen in $\mathscr{F}$

For simplicity, we shall reason in one dimension.

Let $\xi^{(\varepsilon)}_{x_0}(x)$ be a sufficiently regular real function, such that $\int_{-\infty}^{+\infty} dx\ \xi^{(\varepsilon)}_{x_0}(x) = 1$, and having the form of a peak of width ε and amplitude $1/\varepsilon$, centered at $x = x_0$ [see fig. 1; $\xi^{(\varepsilon)}_{x_0}(x)$ is, for example, one of the functions considered in § 1-b of appendix II]. If $\varepsilon \neq 0$, $\xi^{(\varepsilon)}_{x_0}(x) \in \mathscr{F}_x$ (the square of its norm is of the order of $1/\varepsilon$). Denote by $|\ \xi^{(\varepsilon)}_{x_0}\ \rangle$ the corresponding ket:

$$\xi^{(\varepsilon)}_{x_0}(x) \Longleftrightarrow |\ \xi^{(\varepsilon)}_{x_0}\ \rangle \tag{B-13}$$

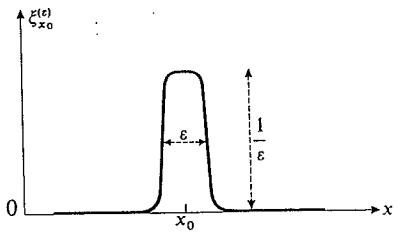

FIGURE 1

$\xi^{(\varepsilon)}_{x_0}(x)$ is a function which has a peak at $x = x_0$ (of width ε and amplitude $1/\varepsilon$), whose integral between $-\infty$ and $+\infty$ is equal to 1.

If $\varepsilon \neq 0$, $|\ \xi^{(\varepsilon)}_{x_0}\ \rangle \in \mathscr{E}_x$. Let $\langle\ \xi^{(\varepsilon)}_{x_0}\ |$ be the bra associated with this ket; for every $|\ \psi\ \rangle \in \mathscr{E}_x$, we have:

$$\langle\ \xi^{(\varepsilon)}_{x_0}\ |\ \psi\ \rangle = (\xi^{(\varepsilon)}_{x_0}, \psi) = \int_{-\infty}^{+\infty} dx\ \xi^{(\varepsilon)}_{x_0}(x)\ \psi(x) \tag{B-14}$$

Now let ε approach zero. On the one hand:

$$\lim_{\varepsilon \to 0} \xi^{(\varepsilon)}_{x_0}(x) = \xi_{x_0}(x) \notin \mathscr{F}_x \tag{B-15}$$

[the square of the norm of $\xi^{(\varepsilon)}_{x_0}(x)$, which is of the order of $1/\varepsilon$, diverges when $\varepsilon \longrightarrow 0$]; therefore:

$$\lim_{\varepsilon \to 0} |\ \xi^{(\varepsilon)}_{x_0}\ \rangle \notin \mathscr{E}_x \tag{B-16}$$

On the other hand, when $\varepsilon \longrightarrow 0$, integral (B-14) approaches a perfectly well-defined limit, $\psi(x_0)$ [since, for sufficiently small ε, $\psi(x)$ can be replaced in (B-14) by $\psi(x_0)$ and removed from the integral]. Consequently, $\langle\ \xi^{(\varepsilon)}_{x_0}\ |$ approaches a bra which we shall denote by $\langle\ \xi_{x_0}\ |$: $\langle\ \xi_{x_0}\ |$ is the linear functional which associates, with every ket $|\ \psi\ \rangle$ of $\mathscr{E}_x$, the value $\psi(x_0)$ taken on by the associated wave function at the point x_0:

$$\lim_{\varepsilon \to 0} \langle\ \xi^{(\varepsilon)}_{x_0}\ | = \langle\ \xi_{x_0}\ | \in \mathscr{E}^*_x$$
$$\text{If } |\ \psi\ \rangle \in \mathscr{E}_x, \langle\ \xi_{x_0}\ |\ \psi\ \rangle = \psi(x_0) \tag{B-17}$$

Thus we see that *the bra* $\langle\ \xi_{x_0}\ |$ *exists, but no ket corresponds to it.*

In the same way, let us consider a plane wave which is truncated outside an interval of width L:

$$v^{(L)}_{p_0}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_0 x/\hbar} \quad \text{if } -\frac{L}{2} \leqslant x \leqslant +\frac{L}{2} \tag{B-18}$$

with the function $v^{(L)}_{p_0}(x)$ going rapidly to zero outside this interval (while remaining continuous and differentiable). We shall denote by $|\ v^{(L)}_{p_0}\ \rangle$ the ket associated with $v^{(L)}_{p_0}(x)$:

$$v^{(L)}_{p_0}(x) \in \mathscr{F}_x \Longleftrightarrow |\ v^{(L)}_{p_0}\ \rangle \in \mathscr{E}_x \tag{B-19}$$

The square of the norm of $v^{(L)}_{p_0}$, which is practically equal to $L/2\pi\hbar$, diverges if $L \longrightarrow \infty$. Therefore:

$$\lim_{L \to \infty} |\ v^{(L)}_{p_0}\ \rangle \notin \mathscr{E}_x \tag{B-20}$$

Now let us consider the bra $\langle\ v^{(L)}_{p_0}\ |$ associated with $|\ v^{(L)}_{p_0}\ \rangle$. For every $|\ \psi\ \rangle \in \mathscr{E}_x$, we have

$$\langle\ v^{(L)}_{p_0}\ |\ \psi\ \rangle = (v^{(L)}_{p_0}, \psi) \simeq \frac{1}{\sqrt{2\pi\hbar}} \int_{-L/2}^{L/2} dx\ e^{-ip_0 x/\hbar} \psi(x) \tag{B-21}$$

When $L \longrightarrow \infty$, $\langle\ v^{(L)}_{p_0}\ |\ \psi\ \rangle$ has a limit: the value $\bar{\psi}(p_0)$ of the Fourier transform $\bar{\psi}(p)$ c $\psi(x)$ for $p = p_0$. Therefore, when $L \longrightarrow \infty$, $\langle\ v^{(L)}_{p_0}\ |$ tends towards a perfectly, well-define bra $\langle\ v_{p_0}\ |$:

$$\lim_{L \to \infty} \langle\ v^{(L)}_{p_0}\ | = \langle\ v_{p_0}\ | \in \mathscr{E}^*_x$$
$$\text{If } |\ \psi\ \rangle \in \mathscr{E}_x, \langle\ v_{p_0}\ |\ \psi\ \rangle = \bar{\psi}(p_0) \tag{B-22}$$

Here again, *no ket corresponds to the bra* $\langle\ v_{p_0}\ |$.

(*ii*) Physical resolution of the preceding difficulties

This dissymmetry of the correspondence between kets and bras is related, as the precedin examples show, to the existence of "continuous bases" for $\mathscr{F}_x$. Since the functions constitutin these "bases" do not belong to $\mathscr{F}_x$, we cannot associate a ket of $\mathscr{E}_x$ with them. However, thei scalar product with an arbitrary function of $\mathscr{F}_x$ is defined, and this permits us to associat with them a linear functional in $\mathscr{E}_x$, that is, a bra belonging to $\mathscr{E}^*_x$. The reason for using suc "continuous bases" lies in their usefulness in certain practical calculations. The same reaso (which will become more apparent in what follows) leads us here to reestablish the symmetr between kets and bras by introducing "generalized kets", defined using functions which are nc square-integrable, but whose scalar product with every function of $\mathscr{F}_x$ exists. In what follow we shall work with "kets" such as $|\ \xi_{x_0}\ \rangle$ or $|\ v_{p_0}\ \rangle$, associated with $\xi_{x_0}(x)$ or $v_{p_0}(x)$. It must nc be forgotten that these generalized "kets" cannot, strictly speaking, represent physical state They are merely intermediaries, useful in calculations involving certain operations which w shall have to perform on the true kets of the space $\mathscr{E}_x$, which actually characterize realizabl quantum states.

This method poses a certain number of mathematical problems, which can be avoide by adopting the following physical point of view: $|\ \xi_{x_0}\ \rangle$ (or $|\ v_{p_0}\ \rangle$) actually denotes $|\ \xi^{(\varepsilon)}_{x_0}$ (or $|\ v^{(L)}_{p_0}\ \rangle$) where ε is very small (or L is very large) compared to all the other lengths in th problem we are considering. In all the intermediary calculations where $|\ \xi^{(\varepsilon)}_{x_0}\ \rangle$ (or $|\ v^{(L)}_{p_0}$ appears, the limit $\varepsilon = 0$ (or $L \longrightarrow \infty$) is never attained, so that one is always working in $\mathscr{E}$ The physical result obtained at the end of the calculation depends very little on the value of as long as ε is sufficiently small with respect to all the other lengths: it is then possible to neglect that is, to set $\varepsilon = 0$, in the final result (the procedure to be used for L is analogous).

The objection could be raised that, unlike $\{\ \xi_{x_0}(x)\ \}$ and $\{\ v_{p_0}(x)\ \}$, $\{\ \xi^{(\varepsilon)}_{x_0}(x)\ \}$ and $\{\ v^{(L)}_{p_0}(x)$ are not orthonormal bases, insofar as they do not rigorously satisfy the closure relation. I fact, they fulfill it approximately. For example, the expression $\int dx_0\ \xi^{(\varepsilon)}_{x_0}(x)\xi^{(\varepsilon)}_{x_0}(x')$ is a functio of $(x - x')$ which can serve as an excellent approximation for $\delta(x - x')$. Its graphical repre sentation is practically a triangle of base 2ε and height $\frac{1}{\varepsilon}$, centered at $x - x' = 0$ (appendix I § 1-c-iv). If ε is negligible compared to all the other lengths in the problem, the difference betwee this expression and $\delta(x - x')$ is physically inappreciable.

In general, the dual space $\mathscr{E}^*$ and the state space $\mathscr{E}$ are not isomorphic, except, of course, if $\mathscr{E}$ is finite-dimensional*: although to each ket $|\psi\rangle$ of $\mathscr{E}$ there corresponds a bra $\langle\psi|$ in $\mathscr{E}^*$, the converse is not true. Nevertheless, we shall agree to use, in addition to vectors belonging to $\mathscr{E}$ (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 $\langle\varphi|$ of $\mathscr{E}^*$, there will correspond a ket. But generalized kets do not represent physical states of the system.

3. Linear operators

a. DEFINITIONS

These are the same as those of § A-1-c.

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

$$|\psi'\rangle = A\,|\psi\rangle \tag{B-23}$$

$$A(\lambda_1\,|\psi_1\rangle + \lambda_2\,|\psi_2\rangle) = \lambda_1 A\,|\psi_1\rangle + \lambda_2 A\,|\psi_2\rangle \tag{B-24}$$

The product of two linear operators A and B, written AB, is defined in the following way:

$$(AB)\,|\psi\rangle = A(B\,|\psi\rangle) \tag{B-25}$$

B first acts on $|\psi\rangle$ to give the ket $B\,|\psi\rangle$; A then acts on the ket $B\,|\psi\rangle$. In general, $AB \neq BA$. The commutator $[A, B]$ of A and B is, by definition:

$$[A, B] = AB - BA \tag{B-26}$$

Let $|\varphi\rangle$ and $|\psi\rangle$ be two kets. We call the *matrix element* of A between $|\varphi\rangle$ and $|\psi\rangle$, the scalar product:

$$\langle\varphi|(A\,|\psi\rangle) \tag{B-27}$$

Consequently, this is *a number* which depends linearly on $|\psi\rangle$ and antilinearly on $|\varphi\rangle$.

b. EXAMPLES OF LINEAR OPERATORS: PROJECTORS

α. *Important comment about Dirac notation*

We have begun to sense, in the preceding, the simplicity and convenience of the Dirac formalism. For example, $\langle\varphi|$ denotes a linear functional (a bra), and $\langle\psi_1\,|\psi_2\rangle$, the scalar product of two kets $|\psi_1\rangle$ and $|\psi_2\rangle$. The number associated by the linear functional $\langle\varphi|$ with an arbitrary ket $|\psi\rangle$ is then written simply by juxtaposing the symbols $\langle\varphi|$ and $|\psi\rangle$: $\langle\varphi\,|\psi\rangle$. This is the scalar product of $|\psi\rangle$ by the ket $|\varphi\rangle$ corresponding to $\langle\varphi|$ (which is why it is useful to have a one-to-one correspondence between kets and bras).

* It is true that the Hilbert space L^2 and its dual space are isomorphic; however, we have taken for the wave function space $\mathscr{F}$ a subspace of L^2, which explains why $\mathscr{F}^*$ is "larger" than $\mathscr{F}$.

Now assume that we write $\langle\varphi|$ and $|\psi\rangle$ in the opposite order:

$$|\psi\rangle\langle\varphi| \tag{B-28}$$

We shall see that if we abide by the rule of juxtaposition of symbols, this expression represents an operator. Choose an arbitrary ket $|\chi\rangle$ and consider:

$$|\psi\rangle\langle\varphi\,|\chi\rangle \tag{B-29}$$

We already know that $\langle\varphi\,|\chi\rangle$ is a complex number; consequently, (B-29) is a ket, obtained by multiplying $|\psi\rangle$ by the scalar $\langle\varphi\,|\chi\rangle$. $|\psi\rangle\langle\varphi|$, applied to an arbitrary ket, gives another ket: it is an operator.

Thus we see that *the order of the symbols is of critical importance.* Only complex numbers can be moved about with impunity, because of the linearity of the space $\mathscr{E}$ and of the operators which we shall use. Indeed, if λ is a number:

$$\begin{cases} |\psi\rangle\lambda = \lambda\,|\psi\rangle \\ \langle\psi\,|\lambda = \lambda\langle\psi| \\ A\lambda\,|\psi\rangle = \lambda A\,|\psi\rangle \qquad \text{(where } A \text{ is a linear operator)} \\ \langle\varphi\,|\lambda\,|\psi\rangle = \lambda\langle\varphi\,|\psi\rangle = \langle\varphi\,|\psi\rangle\lambda \end{cases} \tag{B-30}$$

But, for kets, bras and operators, the order must always be carefully respected in writing the formulas: this is the price that must be paid for the simplicity of the Dirac formalism.

β. *The projector P_ψ onto a ket $|\psi\rangle$*

Let $|\psi\rangle$ be a ket which is normalized to one:

$$\langle\psi\,|\psi\rangle = 1 \tag{B-31}$$

Consider the operator P_ψ defined by:

$$P_\psi = |\psi\rangle\langle\psi| \tag{B-32}$$

and apply it to an arbitrary ket $|\varphi\rangle$:

$$P_\psi\,|\varphi\rangle = |\psi\rangle\langle\psi\,|\varphi\rangle \tag{B-33}$$

P_ψ, acting on an arbitrary ket $|\varphi\rangle$, gives a ket proportional to $|\psi\rangle$. The coefficient of proportionality $\langle\psi\,|\varphi\rangle$ is the scalar product of $|\varphi\rangle$ by $|\psi\rangle$.

The "geometrical" significance of P_ψ is therefore clear: it is the "orthogonal projection" operator onto the ket $|\psi\rangle$.

This interpretation is confirmed by the fact that $P_\psi^2 = P_\psi$ (projecting twice in succession onto a given vector is equivalent to projecting a single time). To see this, we write:

$$P_\psi^2 = P_\psi P_\psi = |\psi\rangle\langle\psi\,|\psi\rangle\langle\psi| \tag{B-34}$$

In this expression, $\langle\psi\,|\psi\rangle$ is a number, which is equal to 1 [formula (B-31)]. Therefore:

$$P_\psi^2 = |\psi\rangle\langle\psi| = P_\psi \tag{B-35}$$

γ. *Projector onto a subspace*

Let $|\varphi_1\rangle, |\varphi_2\rangle, ..., |\varphi_q\rangle$, be q normalized vectors which are orthogonal to each other:

$$\langle \varphi_i | \varphi_j \rangle = \delta_{ij} \quad ; \quad i,j = 1, 2, ..., q \tag{B-36}$$

We denote by $\mathscr{E}_q$ the subspace of $\mathscr{E}$ spanned by these q vectors.

Let P_q be the linear operator defined by:

$$P_q = \sum_{i=1}^{q} |\varphi_i\rangle\langle\varphi_i| \tag{B-37}$$

Calculating P_q^2:

$$P_q^2 = \sum_{i=1}^{q}\sum_{j=1}^{q} |\varphi_i\rangle\langle\varphi_i|\varphi_j\rangle\langle\varphi_j| \tag{B-38}$$

we get, using (B-36):

$$P_q^2 = \sum_{i=1}^{q}\sum_{j=1}^{q} |\varphi_i\rangle\langle\varphi_j|\delta_{ij} = \sum_{i=1}^{q} |\varphi_i\rangle\langle\varphi_i| = P_q \tag{B-39}$$

P_q is therefore a projector. It is easy to see that P_q projects onto the subspace $\mathscr{E}_q$, since for any $|\psi\rangle \in \mathscr{E}$:

$$P_q|\psi\rangle = \sum_{i=1}^{q} |\varphi_i\rangle\langle\varphi_i|\psi\rangle \tag{B-40}$$

P_q acting on $|\psi\rangle$ gives the linear superposition of the projections of $|\psi\rangle$ onto the various $|\varphi_i\rangle$, that is, the projection of $|\psi\rangle$ onto the subspace $\mathscr{E}_q$.

4. Hermitian conjugation

a. ACTION OF A LINEAR OPERATOR ON A BRA

Until now, we have only defined the action of a linear operator A on kets. We are now going to see that it is also possible to define the action of A on bras.

Let $\langle\varphi|$ be a well-defined bra, and consider the set of all kets $|\psi\rangle$. With each of these kets can be associated the complex number $\langle\varphi|(A|\psi\rangle)$, already defined above as the matrix element of A between $|\varphi\rangle$ and $|\psi\rangle$. Since A is linear and the scalar product depends linearly on the ket, the number $\langle\varphi|(A|\psi\rangle)$ depends linearly on $|\psi\rangle$. Thus, for fixed $\langle\varphi|$ and A, we can associate with every ket $|\psi\rangle$ a number which depends linearly on $|\psi\rangle$. The specification of $\langle\varphi|$ and A therefore defines a new linear functional on the kets of $\mathscr{E}$, that is, a new bra belonging to $\mathscr{E}^*$. We shall denote this new bra by $\langle\varphi|A$. The relation which defines $\langle\varphi|A$ can thus be written:

$$\boxed{(\langle\varphi|A)|\psi\rangle = \langle\varphi|(A|\psi\rangle)} \tag{B-41}$$

The operator A associates with every bra $\langle\varphi|$ a new bra $\langle\varphi|A$. Let u show that the correspondence is linear. In order to do this, consider a linea combination of bras $\langle\varphi_1|$ and $\langle\varphi_2|$:

$$\langle\chi| = \lambda_1\langle\varphi_1| + \lambda_2\langle\varphi_2| \tag{B-4}$$

(which means that $\langle\chi|\psi\rangle = \lambda_1\langle\varphi_1|\psi\rangle + \lambda_2\langle\varphi_2|\psi\rangle$). From (B-41), v have:

$$\begin{aligned}(\langle\chi|A)|\psi\rangle &= \langle\chi|(A|\psi\rangle)\\ &= \lambda_1\langle\varphi_1|(A|\psi\rangle) + \lambda_2\langle\varphi_2|(A|\psi\rangle)\\ &= \lambda_1(\langle\varphi_1|A)|\psi\rangle + \lambda_2(\langle\varphi_2|A)|\psi\rangle\end{aligned} \tag{B-4}$$

Since $|\psi\rangle$ is arbitrary, it follows that:

$$\begin{aligned}\langle\chi|A &= (\lambda_1\langle\varphi_1| + \lambda_2\langle\varphi_2|)A\\ &= \lambda_1\langle\varphi_1|A + \lambda_2\langle\varphi_2|A\end{aligned} \tag{B-4}$$

Equation (B-41) therefore defines a linear operation on bras. The b $\langle\varphi|A$ is the bra which results from the action of the linear operator A c the bra $\langle\varphi|$.

COMMENTS:

(*i*) From definition (B-41) of $\langle\varphi|A$, we see that the place of the parenthes in the symbol defining the matrix element of A between $|\varphi\rangle$ and $|\psi$ is of no importance. Therefore, we shall henceforth designate this matr element by the notation $\langle\varphi|A|\psi\rangle$:

$$\langle\varphi|A|\psi\rangle = (\langle\varphi|A)|\psi\rangle = \langle\varphi|(A|\psi\rangle) \tag{B-4}$$

(*ii*) The relative order of $\langle\varphi|$ and A is very important in the notatic $\langle\varphi|A$ (*cf.* § 3-b-α above). One must write $\langle\varphi|A$ and not $A\langle\varphi|$: $\langle\varphi|$ acting on a ket $|\psi\rangle$ gives a number $\langle\varphi|A|\psi\rangle$; $\langle\varphi|A$ is therefore inde a bra. On the other hand, $A\langle\varphi|$, acting on a ket $|\psi\rangle$, would gi $A\langle\varphi|\psi\rangle$, that is, an operator (the operator A multiplied by the numb $\langle\varphi|\psi\rangle$). We have not defined any mathematical object of this sor $A\langle\varphi|$ therefore has no meaning.

b. THE ADJOINT OPERATOR $A^\dagger$ OF A LINEAR OPERATOR A

We are now going to see that the correspondence between kets and bra studied in § B-2-c, enables us to associate with every linear operator A anoth linear operator $A^\dagger$, called the adjoint operator (or Hermitian conjugate) of .

Let $|\psi\rangle$ then be an arbitrary ket of $\mathscr{E}$. The operator A associates with another ket $|\psi'\rangle = A|\psi\rangle$ of $\mathscr{E}$ (fig. 2).

To the ket $|\psi\rangle$ corresponds a bra $\langle\psi|$; in the same way, to $|\psi'\rangle$ cc responds $\langle\psi'|$. This correspondence between kets and bras thus permits us to defi the action of the operator $A^\dagger$ on the bras: the operator $A^\dagger$ associates with t bra $\langle\psi|$ corresponding to the ket $|\psi\rangle$, the bra $\langle\psi'|$ corresponding to t ket $|\psi'\rangle = A|\psi\rangle$. We write: $\langle\psi'| = \langle\psi|A^\dagger$.

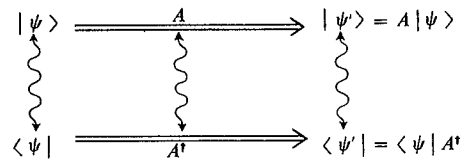

FIGURE 2

Definition of the adjoint operator $A^\dagger$ of an operator A using the correspondence between kets and bras.

Let us show that the relation $\langle\psi'| = \langle\psi|A^\dagger$ is linear. We know that, to the bra $\lambda_1\langle\psi_1| + \lambda_2\langle\psi_2|$, corresponds the ket $\lambda_1^*|\psi_1\rangle + \lambda_2^*|\psi_2\rangle$ (the correspondence between a bra and a ket is antilinear). The operator A transforms $\lambda_1^*|\psi_1\rangle + \lambda_2^*|\psi_2\rangle$ into $\lambda_1^*A|\psi_1\rangle + \lambda_2^*A|\psi_2\rangle = \lambda_1^*|\psi_1'\rangle + \lambda_2^*|\psi_2'\rangle$. Finally, to this ket corresponds the bra:

$$\lambda_1\langle\psi_1'| + \lambda_2\langle\psi_2'| = \lambda_1\langle\psi_1|A^\dagger + \lambda_2\langle\psi_2|A^\dagger.$$

From this we conclude that:

$$(\lambda_1\langle\psi_1| + \lambda_2\langle\psi_2|)A^\dagger = \lambda_1\langle\psi_1|A^\dagger + \lambda_2\langle\psi_2|A^\dagger \tag{B-46}$$

$A^\dagger$ is therefore a linear operator, defined by the formula:

$$\boxed{|\psi'\rangle = A|\psi\rangle \Longleftrightarrow \langle\psi'| = \langle\psi|A^\dagger} \tag{B-47}$$

From (B-47), it is easy to deduce another important relationship satisfied by the operator $A^\dagger$. Using the properties of the scalar product, one can always write:

$$\langle\psi'|\varphi\rangle = \langle\varphi|\psi'\rangle^* \tag{B-48}$$

where $|\varphi\rangle$ is an arbitrary ket of $\mathcal{E}$. Using expressions (B-47) for $|\psi'\rangle$ and $\langle\psi'|$, we obtain:

$$\boxed{\langle\psi|A^\dagger|\varphi\rangle = \langle\varphi|A|\psi\rangle^*} \tag{B-49}$$

a relation which is valid for all $|\varphi\rangle$ and $|\psi\rangle$.

COMMENT ABOUT NOTATION

We have already mentioned a notation which can lead to confusion: $|\lambda\psi\rangle$ and $\langle\lambda\psi|$, where λ is a scalar [formulas (B-7) and (B-8)]. The same problem arises with the expressions $|A\psi\rangle$ and $\langle A\psi|$, where A is a linear operator. $|A\psi\rangle$ is another way of designating the ket $A|\psi\rangle$:

$$|A\psi\rangle = A|\psi\rangle \tag{B-50}$$

$\langle A\psi|$ is the bra associated with the ket $|A\psi\rangle$. Using (B-50) and (B-47), we see that:

$$\langle A\psi| = \langle\psi|A^\dagger \tag{B-51}$$

When a linear operator A is taken outside the bra symbol, it must be replaced by its adjoint $A^\dagger$ (and placed to the right of the bra).

c. CORRESPONDENCE BETWEEN AN OPERATOR AND ITS ADJOINT

By using (B-47) or (B-49), it is easy to show that

$$(A^\dagger)^\dagger = A \tag{B-52}$$

$$(\lambda A)^\dagger = \lambda^* A^\dagger \qquad \text{(where } \lambda \text{ is a number)} \tag{B-53}$$

$$(A + B)^\dagger = A^\dagger + B^\dagger \tag{B-54}$$

Now let us calculate $(AB)^\dagger$. To do this, consider the ket $|\varphi\rangle = AB|\psi\rangle$. Write it in the form $|\varphi\rangle = A|\chi\rangle$, setting $|\chi\rangle = B|\psi\rangle$. Then:

$$\langle\varphi| = \langle\psi|(AB)^\dagger = \langle\chi|A^\dagger = \langle\psi|B^\dagger A^\dagger$$

since $\langle\chi| = \langle\psi|B^\dagger$. From this, we deduce that:

$$\boxed{(AB)^\dagger = B^\dagger A^\dagger} \tag{B-55}$$

Note that *the order changes when one takes the adjoint of a product of operators.*

COMMENT:

Since $(A^\dagger)^\dagger = A$, we can write, using (B-51):

$$\langle A^\dagger\varphi| = \langle\varphi|(A^\dagger)^\dagger = \langle\varphi|A$$

Thus the left-hand side of (B-41) can be rewritten in the form $\langle A^\dagger\varphi|\psi\rangle$. In the same way, the right-hand side of this same equation can be put, with the notation of (B-50), into the form $\langle\varphi|A\psi\rangle$. From this results the following equation, sometimes used to define the adjoint operator $A^\dagger$ of A:

$$\langle A^\dagger\varphi|\psi\rangle = \langle\varphi|A\psi\rangle \tag{B-56}$$

d. HERMITIAN CONJUGATION IN DIRAC NOTATION

In the preceding section, we introduced the concept of an adjoint operator by using the correspondence between kets and bras. A ket $|\psi\rangle$ and its corresponding bra $\langle\psi|$ are said to be "Hermitian conjugates" of each other. The operation of Hermitian conjugation is represented by the wavy arrows in figure 2; we see that it associates $A^\dagger$ with A. This is the reason why $A^\dagger$ is also called the Hermitian conjugate operator of A.

The operation of Hermitian conjugation changes the order of the objects to which it is applied. Thus we see in figure 2 that $A|\psi\rangle$ becomes $\langle\psi|A^\dagger$. The ket $|\psi\rangle$ is changed into $\langle\psi|$, and A into $A^\dagger$. Moreover, the order is reversed. In the same way, we saw in (B-55) that the Hermitian conjugate of a product of two operators is equal to the product of the Hermitian conjugates taken in the opposite order. Finally, let us show that:

$$(|u\rangle\langle v|)^\dagger = |v\rangle\langle u| \tag{B-57}$$

($|u\rangle$ is replaced by $\langle u|$, and $\langle v|$ by $|v\rangle$, and the order is changed). Applying relation (B-49) to the operator $|u\rangle\langle v|$, we find:

$$\langle\psi|(|u\rangle\langle v|)^\dagger|\varphi\rangle = [\langle\varphi|(|u\rangle\langle v|)|\psi\rangle]^* \tag{B-58}$$

Now, if we use property (B-9) of the scalar product:

$$[\langle \varphi | (|u\rangle\langle v|) | \psi \rangle]^* = \langle \varphi | u \rangle^* \langle v | \psi \rangle^* = \langle \psi | v \rangle \langle u | \varphi \rangle$$
$$= \langle \psi | (|v\rangle\langle u|) | \varphi \rangle \qquad \text{(B-59)}$$

By comparing (B-58) and (B-59), we can derive (B-57).

The result of the operation of Hermitian conjugation on a constant remains to be found. We see from (B-6) and (B-53) that this operation simply transforms λ into λ^* (complex conjugation). This is in agreement with the fact that $\langle \varphi | \psi \rangle^* = \langle \psi | \varphi \rangle$.

Therefore, the Hermitian conjugate of a ket is a bra, and vice versa; that of an operator is its adjoint; that of a number, its complex conjugate. In Dirac notation, the operation of Hermitian conjugation is very simple to perform; it suffices to apply the following rule:

RULE

To obtain the Hermitian conjugate (or the adjoint) of any expression composed of constants, kets, bras and operators, one must:

- *Replace* { the constants by their complex conjugates; the kets by the bras associated with them; the bras by the kets associated with them; the operators by their adjoints }
- *Reverse the order* of the factors (the position of the constants, nevertheless, is of no importance).

EXAMPLES

$\lambda \langle u | A | v \rangle | w \rangle \langle \psi |$ is an operator (λ and $\langle u | A | v \rangle$ are numbers). The adjoint of this operator is obtained by using the preceding rule: $| \psi \rangle \langle w | \langle v | A^\dagger | u \rangle \lambda^*$, which can also be written $\lambda^* \langle v | A^\dagger | u \rangle | \psi \rangle \langle w |$, changing the position of the numbers λ^* and $\langle v | A^\dagger | u \rangle$.

In the same way, $\lambda | u \rangle \langle v | w \rangle$ is a ket (λ and $\langle v | w \rangle$ are constants). The conjugate bra is $\langle w | v \rangle \langle u | \lambda^*$, which can also be written $\lambda^* \langle w | v \rangle \langle u |$.

e. HERMITIAN OPERATORS

An operator A is said to be Hermitian if it is equal to its adjoint, that is, if:

$$A = A^\dagger \qquad \text{(B-60)}$$

Combining (B-60) and (B-49), we see that a Hermitian operator satisfies the relation:

$$\langle \psi | A | \varphi \rangle = \langle \varphi | A | \psi \rangle^* \qquad \text{(B-61)}$$

which is valid for all $| \varphi \rangle$ and $| \psi \rangle$.

Finally, for a Hermitian operator, (B-56) becomes

$$\langle A\varphi | \psi \rangle = \langle \varphi | A\psi \rangle \qquad \text{(B-62)}$$

We shall treat Hermitian operators in more detail later, when we consider the problem of eigenvalues and eigenvectors. Moreover, we shall see in chapter III that Hermitian operators play a fundamental role in quantum mechanics.

If formula (B-57) is applied to the case where $|u\rangle = |v\rangle = |\psi\rangle$, we see that the projector $P_\psi = |\psi\rangle\langle\psi|$ is Hermitian:

$$P_\psi^\dagger = |\psi\rangle\langle\psi| = P_\psi \qquad \text{(B-63)}$$

COMMENT:

The product of two Hermitian operators A and B is Hermitian only if $[A, B] = 0$. Indeed, if $A = A^\dagger$ and $B = B^\dagger$, it can be shown using (B-55) that $(AB)^\dagger = B^\dagger A^\dagger = BA$, which is equal to AB only if $[A, B] = 0$.

C. REPRESENTATIONS IN STATE SPACE

1. Introduction

a. DEFINITION OF A REPRESENTATION

Choosing a representation means choosing an orthonormal basis, either discrete or continuous, 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. The vectorial calculus introduced in § B then becomes a matrix calculus with these numbers. The choice of a representation is, in theory, arbitrary. Actually, it obviously depends on the particular problem being studied: in each case, one chooses the representation which leads to the simplest calculations.

b. AIM OF SECTION C

Using the Dirac notation, and for any arbitrary $\mathscr{E}$ space, we are going to treat again all the concepts introduced in §§ A-2 and A-3 for discrete and continuous bases of $\mathscr{F}$.

We shall write the two characteristic relations of a basis in Dirac notation: the orthonormalization and closure relations. Then we shall show how, using these two relations, it is possible to solve all specific problems involving a representation and the transformation from one representation to another.

2. Relations characteristic of an orthonormal basis

a. ORTHONORMALIZATION RELATION

A set of kets, discrete ($\{ |u_i\rangle \}$) or continuous ($\{ |w_\alpha\rangle \}$), is said to be *orthonormal* if the kets of this set satisfy the orthonormalization relation:

$$\langle u_i | u_j \rangle = \delta_{ij} \qquad \text{(C-1)}$$

or

$$\boxed{\langle w_\alpha | w_{\alpha'} \rangle = \delta(\alpha - \alpha')} \tag{C-2}$$

It can be seen that, for a continuous set, $\langle w_\alpha | w_\alpha \rangle$ does not exist: the $|w_\alpha\rangle$ have an infinite norm and therefore do not belong to $\mathcal{E}$. Nevertheless, the vectors of $\mathcal{E}$ can be expanded on the $|w_\alpha\rangle$. It is useful, consequently, to accept the $|w_\alpha\rangle$ as generalized kets (see the discussions in §§ A-3 and B-2-c).

b. CLOSURE RELATION

A discrete set, $\{|u_i\rangle\}$, or a continuous one, $\{|w_\alpha\rangle\}$, constitutes a *basis* if every ket $|\psi\rangle$ belonging to $\mathcal{E}$ has a unique expansion on the $|u_i\rangle$ or the $|w_\alpha\rangle$

$$\boxed{|\psi\rangle = \sum_i c_i |u_i\rangle} \tag{C-3}$$

$$\boxed{|\psi\rangle = \int d\alpha\ c(\alpha) |w_\alpha\rangle} \tag{C-4}$$

Let us assume, moreover, that the basis is orthonormal. Then perform the scalar multiplication on both sides of (C-3) with $\langle u_j|$, and on both sides of (C-4) with $\langle w_{\alpha'}|$. We obtain, using (C-1) or (C-2), expressions for the components c_j or $c(\alpha')$:

$$\langle u_j | \psi \rangle = c_j \tag{C-5}$$

$$\langle w_{\alpha'} | \psi \rangle = c(\alpha') \tag{C-6}$$

Then replace in (C-3) c_i by $\langle u_i|\psi\rangle$, and in (C-4) $c(\alpha)$ by $\langle w_\alpha|\psi\rangle$:

$$|\psi\rangle = \sum_i c_i |u_i\rangle = \sum_i \langle u_i | \psi \rangle |u_i\rangle$$
$$= \sum_i |u_i\rangle\langle u_i| \psi\rangle = \left(\sum_i |u_i\rangle\langle u_i|\right)|\psi\rangle \tag{C-7}$$

$$|\psi\rangle = \int d\alpha\ c(\alpha)|w_\alpha\rangle = \int d\alpha \langle w_\alpha|\psi\rangle |w_\alpha\rangle$$
$$= \int d\alpha |w_\alpha\rangle\langle w_\alpha|\psi\rangle = \left(\int d\alpha |w_\alpha\rangle\langle w_\alpha|\right)|\psi\rangle \tag{C-8}$$

[since, in (C-7), we can place the number $\langle u_i|\psi\rangle$ after the ket $|u_i\rangle$; in the same way, in (C-8), we can place the number $\langle w_\alpha|\psi\rangle$ after the ket $|w_\alpha\rangle$].

Thus, we see two operators appear, $\sum_i |u_i\rangle\langle u_i|$ and $\int d\alpha |w_\alpha\rangle\langle w_\alpha|$. They

act on every ket $|\psi\rangle$ belonging to $\mathcal{E}$ to give the same ket $|\psi\rangle$. Since $|\psi\rangle$ is arbitrary, it follows that:

$$\boxed{P_{\{u_i\}} = \sum_i |u_i\rangle\langle u_i| = \mathbb{1}} \tag{C-9}$$

$$\boxed{P_{\{w_\alpha\}} = \int d\alpha |w_\alpha\rangle\langle w_\alpha| = \mathbb{1}} \tag{C-10}$$

where $\mathbb{1}$ denotes the identity operator in $\mathcal{E}$. Relation (C-9), or (C-10), is called the *closure relation*. Conversely, let us show that relations (C-9) and (C-10) express the fact that the sets $\{|u_i\rangle\}$ and $\{|w_\alpha\rangle\}$ constitute bases. For every $|\psi\rangle$ belonging to $\mathcal{E}$, we can write:

$$|\psi\rangle = \mathbb{1}|\psi\rangle = P_{\{u_i\}}|\psi\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle$$
$$= \sum_i c_i |u_i\rangle \tag{C-11}$$

with:

$$c_i = \langle u_i | \psi \rangle \tag{C-12}$$

In the same way:

$$|\psi\rangle = \mathbb{1}|\psi\rangle = P_{\{w_\alpha\}}|\psi\rangle = \int d\alpha |w_\alpha\rangle\langle w_\alpha|\psi\rangle$$
$$= \int d\alpha\ c(\alpha)|w_\alpha\rangle \tag{C-13}$$

with:

$$c(\alpha) = \langle w_\alpha | \psi \rangle \tag{C-14}$$

Thus, every ket $|\psi\rangle$ has a unique expansion on the $|u_i\rangle$ or on the $|w_\alpha\rangle$. Each of these two sets therefore forms a basis, a discrete one or a continuous one. We also see that relation (C-9), or (C-10), spares us the need of memorizing expressions (C-12) and (C-14) for the components c_i and $c(\alpha)$.

COMMENTS:

(*i*) We shall see later (§ E) that, in the case of the $\mathcal{F}$-space, relations (A-32) and (A-57) can easily be deduced from (C-9) and (C-10).

(*ii*) Geometrical interpretation of the closure relation.

From the discussion of § B-3-b, we see that $\sum_i |u_i\rangle\langle u_i|$ is a projector: the projector onto the subspace $\mathcal{E}'$ spanned by $|u_1\rangle, |u_2\rangle, \ldots |u_i\rangle \ldots$ If the $|u_i\rangle$ form a basis, every ket of $\mathcal{E}$ can be expanded on the $|u_i\rangle$; the subspace $\mathcal{E}'$ is then identical with the $\mathcal{E}$-space itself. Consequently, it is reasonable for $\sum_i |u_i\rangle\langle u_i|$ to be equal to the

identity operator : projecting onto $\mathscr{E}$ a ket which belongs to $\mathscr{E}$ does not modify this ket. The same argument can be applied to $\int d\alpha \, |w_\alpha\rangle\langle w_\alpha|$.

We can now find an equivalent of the closure relation for the three-dimensional space of ordinary geometry, R^3. If $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ are three orthonormal vectors of this space, and P_1, P_2 and P_3 are the projectors onto these three vectors, the fact that $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ forms a basis in R^3 is expressed by the relation

$$P_1 + P_2 + P_3 = \mathbb{1} \tag{C-15}$$

On the other hand, $\{\mathbf{e}_1, \mathbf{e}_2\}$ constitutes an orthonormal set but not a basis of R^3. This is expressed by the fact that the projector $P_1 + P_2$ (which projects onto the plane spanned by $\mathbf{e}_1$ and $\mathbf{e}_2$) is not equal to $\mathbb{1}$; for example : $(P_1 + P_2)\mathbf{e}_3 = 0$.

Table (II-7) summarizes the only fundamental formulas which are required for any calculation to be performed in the $\{|u_i\rangle\}$ or $\{|w_\alpha\rangle\}$ representation.

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

Table (II-7)

3. Representation of kets and bras

a. REPRESENTATION OF KETS

In the $\{|u_i\rangle\}$ basis, the ket $|\psi\rangle$ is represented by the set of its components, that is, by the set of numbers $c_i = \langle u_i|\psi\rangle$. These numbers can be arranged vertically to form a one-column matrix (with, in general, a countable infinity of rows):

$$\begin{pmatrix} \langle u_1 \mid \psi \rangle \\ \langle u_2 \mid \psi \rangle \\ \vdots \\ \langle u_i \mid \psi \rangle \\ \vdots \end{pmatrix} \tag{C-16}$$

In the continuous $\{|w_\alpha\rangle\}$ basis, the ket $|\psi\rangle$ is represented by a continuous infinity of numbers, $c(\alpha) = \langle w_\alpha|\psi\rangle$, that is, by a function of α. It is then possible to draw a vertical axis, along which are placed the various possible values of α. To each of these values corresponds a number, $\langle w_\alpha|\psi\rangle$:

$$\alpha \downarrow \begin{pmatrix} \vdots \\ \langle w_\alpha \mid \psi \rangle \\ \vdots \end{pmatrix} \tag{C-17}$$

b. REPRESENTATION OF BRAS

Let $\langle\varphi|$ be an arbitrary bra. In the $\{|u_i\rangle\}$ basis, we can write :

$$\langle\varphi| = \langle\varphi|\mathbb{1} = \langle\varphi|P_{\{u_i\}} = \sum_i \langle\varphi|u_i\rangle\langle u_i| \tag{C-18}$$

$\langle\varphi|$ has a unique expansion on the bras $\langle u_i|$. The components of $\langle\varphi|$, $\langle\varphi|u_i\rangle$, are the complex conjugates of the components $b_i = \langle u_i|\varphi\rangle$ of the ket $|\varphi\rangle$ associated with $\langle\varphi|$.

In the same way, we obtain, in the $\{|w_\alpha\rangle\}$ basis :

$$\langle\varphi| = \langle\varphi|\mathbb{1} = \langle\varphi|P_{\{w_\alpha\}} = \int d\alpha \, \langle\varphi|w_\alpha\rangle\langle w_\alpha| \tag{C-19}$$

The components of $\langle\varphi|$, $\langle\varphi|w_\alpha\rangle$, are the complex conjugates of the components $b(\alpha) = \langle w_\alpha|\varphi\rangle$ of the ket $|\varphi\rangle$ associated with $\langle\varphi|$.

We have agreed to arrange the components of a ket vertically. Before describing how to arrange the components of a bra, let us show how the closure relation enables us to find simply the expression for the scalar product of two kets in terms of their components. We know that we can always place $\mathbb{1}$ between $\langle\varphi|$ and $|\psi\rangle$ in the expression for the scalar product :

$$\begin{aligned} \langle\varphi|\psi\rangle &= \langle\varphi|\mathbb{1}|\psi\rangle = \langle\varphi|P_{\{u_i\}}|\psi\rangle \\ &= \sum_i \langle\varphi|u_i\rangle\langle u_i|\psi\rangle = \sum_i b_i^* c_i \end{aligned} \tag{C-20}$$

In the same way :

$$\begin{aligned} \langle\varphi|\psi\rangle &= \langle\varphi|\mathbb{1}|\psi\rangle = \langle\varphi|P_{\{w_\alpha\}}|\psi\rangle \\ &= \int d\alpha \, \langle\varphi|w_\alpha\rangle\langle w_\alpha|\psi\rangle = \int d\alpha \; b^*(\alpha)\; c(\alpha) \end{aligned} \tag{C-21}$$

Let us arrange the components $\langle\varphi|u_i\rangle$ of the bra $\langle\varphi|$ horizontally, to form a row matrix (having one row and an infinite number of columns) :

$$(\langle\varphi|u_1\rangle \;\; \langle\varphi|u_2\rangle \;\; \ldots\ldots \langle\varphi|u_i\rangle \;\; \ldots\ldots) \tag{C-22}$$

Using this convention, $\langle\varphi|\psi\rangle$ is the matrix product of the column matrix which represents $|\psi\rangle$ and the row matrix which represents $\langle\varphi|$. The result is a matrix having one row and one column, that is, a *number*.

In the $\{|w_\alpha\rangle\}$ basis, $\langle\varphi|$ has a continuous infinity of components $\langle\varphi|w_\alpha\rangle$ The various values of α are placed along a horizontal axis. To each of these values

corresponds a component $\langle \varphi | w_\alpha \rangle$ of $\langle \varphi |$:

$$(\ldots\ldots\ldots \langle \varphi | w_\alpha \rangle \ldots\ldots\ldots) \qquad \alpha \rightarrow \qquad \text{(C-23)}$$

COMMENT:

In a given representation, the matrices which represent a ket $|\psi\rangle$ and the associated bra $\langle \psi |$ are Hermitian conjugates of each other (in the matrix sense): one passes from one matrix to the other by interchanging rows and columns and taking the complex conjugate of each element.

4. Representation of operators

a. REPRESENTATION OF A BY A "SQUARE" MATRIX

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

$$\boxed{A_{ij} = \langle u_i | A | u_j \rangle} \qquad \text{(C-24)}$$

or

$$\boxed{A(\alpha, \alpha') = \langle w_\alpha | A | w_{\alpha'} \rangle} \qquad \text{(C-25)}$$

These numbers depend on two indices and can therefore be arranged in a "square" matrix having a countable or continuous infinity of rows and columns. The usual convention is to have the first index fix the rows and the second, the columns. Thus, in the $\{ |u_i\rangle \}$ basis, the operator A is represented by the matrix:

$$\begin{pmatrix} A_{11} & A_{12} \cdots & A_{1j} & \cdots \\ A_{21} & A_{22} \cdots & A_{2j} & \cdots \\ \vdots & \vdots & \vdots & \\ A_{i1} & A_{i2} \cdots & A_{ij} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \qquad \text{(C-26)}$$

We see that the jth column is made up of the components in the $\{ |u_i\rangle \}$ basis of the transform $A|u_j\rangle$ of the basis vector $|u_j\rangle$.

For a continuous basis, we draw two perpendicular axes. To a point which has for its abscissa α' and for its ordinate α there corresponds the number $A(\alpha, \alpha')$:

$$\alpha' \downarrow \qquad \alpha \rightarrow \left(\begin{array}{c} \vdots \\ \ldots\ldots A(\alpha, \alpha') \end{array} \right) \qquad \text{(C-27)}$$

Let us use the closure relation to calculate the matrix which represents the operator AB in the $\{ |u_i\rangle \}$ basis:

$$\begin{aligned} \langle u_i | AB | u_j \rangle &= \langle u_i | A \mathbb{1} B | u_j \rangle \\ &= \langle u_i | A P_{(u_k)} B | u_j \rangle \\ &= \sum_k \langle u_i | A | u_k \rangle \langle u_k | B | u_j \rangle \end{aligned} \qquad \text{(C-28)}$$

The convention chosen above for the arrangement of the elements A_{ij} [or $A(\alpha, \alpha')$] is therefore consistent with the one relating to the product of two matrices: (C-28) expresses the fact that the matrix representing the operator AB is the product of the matrices associated with A and B.

b. MATRIX REPRESENTATION OF THE KET $|\psi'\rangle = A|\psi\rangle$

The problem is the following: knowing the components of $|\psi\rangle$ and the matrix elements of A in a given representation, how can we calculate the components of $|\psi'\rangle = A|\psi\rangle$ in the same representation?

In the $\{ |u_i\rangle \}$ basis, the coordinate c'_i of $|\psi'\rangle$ are given by:

$$c'_i = \langle u_i | \psi' \rangle = \langle u_i | A | \psi \rangle \qquad \text{(C-29)}$$

If we simply insert the closure relation between A and $|\psi\rangle$, we obtain:

$$\begin{aligned} c'_i &= \langle u_i | A \mathbb{1} | \psi \rangle = \langle u_i | A P_{(u_j)} | \psi \rangle \\ &= \sum_j \langle u_i | A | u_j \rangle \langle u_j | \psi \rangle \\ &= \sum_j A_{ij} c_j \end{aligned} \qquad \text{(C-30)}$$

For the $\{ |w_\alpha\rangle \}$ basis, we obtain, in the same way:

$$\begin{aligned} c'(\alpha) &= \langle w_\alpha | \psi' \rangle = \langle w_\alpha | A | \psi \rangle \\ &= \int d\alpha' \langle w_\alpha | A | w_{\alpha'} \rangle \langle w_{\alpha'} | \psi \rangle \\ &= \int d\alpha' A(\alpha, \alpha') \; c(\alpha') \end{aligned} \qquad \text{(C-31)}$$

The matrix expression for $|\psi'\rangle = A|\psi\rangle$ is therefore very simple. We see, for example from (C-30), that the column matrix representing $|\psi'\rangle$ is equal to the product of the column matrix representing $|\psi\rangle$ and the square matrix representing A:

$$\begin{pmatrix} c'_1 \\ c'_2 \\ \vdots \\ c'_i \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1j} & \cdots \\ A_{21} & A_{22} & \cdots & A_{2j} & \cdots \\ \vdots & \vdots & & \vdots & \\ A_{i1} & A_{i2} & \cdots & A_{ij} & \cdots \\ \vdots & \vdots & & \vdots & \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_j \\ \vdots \end{pmatrix} \tag{C-32}$$

c. EXPRESSION FOR THE NUMBER $\langle \varphi | A | \psi \rangle$

By inserting the closure relation between $\langle \varphi |$ and A and again between A and $|\psi\rangle$, we obtain:

– for the $\{ |u_i\rangle \}$ basis:

$$\begin{aligned} \langle \varphi | A | \psi \rangle &= \langle \varphi | P_{\{u_i\}} A P_{\{u_j\}} | \psi \rangle \\ &= \sum_{i,j} \langle \varphi | u_i \rangle \langle u_i | A | u_j \rangle \langle u_j | \psi \rangle \\ &= \sum_{i,j} b_i^* \; A_{ij} \; c_j \end{aligned} \tag{C-33}$$

– for the $\{ |w_\alpha\rangle \}$ basis:

$$\begin{aligned} \langle \varphi | A | \psi \rangle &= \langle \varphi | P_{\{w_\alpha\}} A P_{\{w_{\alpha'}\}} | \psi \rangle \\ &= \iint d\alpha \, d\alpha' \, \langle \varphi | w_\alpha \rangle \langle w_\alpha | A | w_{\alpha'} \rangle \langle w_{\alpha'} | \psi \rangle \\ &= \iint d\alpha \, d\alpha' \; b^*(\alpha) \; A(\alpha, \alpha') \; c(\alpha') \end{aligned} \tag{C-34}$$

The interpretation of these formulas in the matrix formalism, is as follows: $\langle \varphi | A | \psi \rangle$ is a number, that is, a matrix with one row and one column, obtained by multiplying the column matrix representing $|\psi\rangle$ first by the square matrix representing A and then by the row matrix representing $\langle \varphi |$. For example, in the $\{ |u_i\rangle \}$ basis:

$$\langle \varphi | A | \psi \rangle = (b_1^* \; b_2^* \ldots b_i^* \ldots) \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1j} & \cdots \\ A_{21} & A_{22} & \cdots & A_{2j} & \cdots \\ \vdots & \vdots & & \vdots & \\ A_{i1} & A_{i2} & \cdots & A_{ij} & \cdots \\ \vdots & \vdots & & \vdots & \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_j \\ \vdots \end{pmatrix} \tag{C-35}$$

COMMENTS:

(*i*) It can be shown in the same way that the bra $\langle \varphi | A$ is represented by a row matrix, the product of the square matrix representing A by the row matrix representing $\langle \varphi |$ [the first two matrices of the right-hand side of (C-35)]. Again we see the importance of the order of the symbols: the expression $A \langle \varphi |$ would lead to a matrix operation which is undefined (the product of a row matrix by a square matrix).

(*ii*) From a matrix point of view, equation (B-41) which defines $\langle \varphi | A$ merely expresses the associativity of the product of the three matrices which appear in (C-35).

(*iii*) Using the preceding conventions, we express $|\psi\rangle \langle \psi |$ by a square matrix:

$$\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_i \\ \vdots \end{pmatrix} (c_1^* \; c_2^* \ldots \; c_j^* \ldots) = \begin{pmatrix} c_1 c_1^* & c_1 c_2^* & \cdots & c_1 c_j^* & \cdots \\ c_2 c_1^* & c_2 c_2^* & \cdots & c_2 c_j^* & \cdots \\ \vdots & & & & \\ c_i c_1^* & c_i c_2^* & \cdots & c_i c_j^* & \cdots \\ \vdots & \vdots & & \vdots & \end{pmatrix} \tag{C-36}$$

This is indeed an operator, while $\langle \psi | \psi \rangle$, the product of a column matrix by a row matrix, is a number.

d. MATRIX REPRESENTATION OF THE ADJOINT $A^\dagger$ OF A

Using (B-49), we obtain easily:

$$(A^\dagger)_{ij} = \langle u_i | A^\dagger | u_j \rangle = \langle u_j | A | u_i \rangle^* = A_{ji}^* \tag{C-37}$$

or

$$A^\dagger(\alpha, \alpha') = \langle w_\alpha | A^\dagger | w_{\alpha'} \rangle = \langle w_{\alpha'} | A | w_\alpha \rangle^* = A^*(\alpha', \alpha) \tag{C-38}$$

Therefore, the matrices representing A and $A^\dagger$ in a given representation are Hermitian conjugates of each other, in the matrix sense: *one passes from one to the other by interchanging rows and columns and then taking the complex conjugate.*

If A is Hermitian, $A^\dagger = A$, and we can then replace $(A^\dagger)_{ij}$ by A_{ij} in (C-37), and $A^\dagger(\alpha, \alpha')$ by $A(\alpha, \alpha')$ in (C-38):

$$A_{ij} = A_{ji}^* \tag{C-39}$$

$$A(\alpha, \alpha') = A^*(\alpha', \alpha) \tag{C-40}$$

A Hermitian operator is therefore represented by a Hermitian matrix, that is, one in which *any two elements which are symmetric with respect to the principal diagonal are complex conjugates of each other.* In particular, for $i = j$ or $\alpha = \alpha'$, (C-39) and (C-40) become:

$$A_{ii} = A_{ii}^* \tag{C-41}$$

$$A(\alpha, \alpha) = A^*(\alpha, \alpha) \tag{C-42}$$

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

5. Change of representations

a. OUTLINE OF THE PROBLEM

In a given representation, a ket (or a bra, or an operator) is represented by a matrix. If we change representations, that is, bases, the same ket (or bra, or operator) will be represented by a different matrix. How are these two matrices related?

For the sake of simplicity, we shall assume here that we are going from one discrete orthonormal basis $\{ |u_i\rangle \}$ to another discrete orthonormal basis $\{ |t_k\rangle \}$. In § E, we shall study an example of changing from one continuous basis to another continuous basis.

The change of basis is defined by specifying the components $\langle u_i | t_k \rangle$ of each of the kets of the new basis in terms of each of the kets of the old one. We shall set:

$$S_{ik} = \langle u_i \mid t_k \rangle \tag{C-43}$$

S is the matrix of the basis change (transformation matrix). If $S^\dagger$ denotes its Hermitian conjugate:

$$(S^\dagger)_{ki} = (S_{ik})^* = \langle t_k | u_i \rangle \tag{C-44}$$

The following calculations can be performed very easily, and without memorization, by using the two closure relations:

$$P_{\{u_i\}} = \sum_i |u_i\rangle\langle u_i| = \mathbb{1} \tag{C-45}$$

$$P_{\{t_k\}} = \sum_k |t_k\rangle\langle t_k| = \mathbb{1} \tag{C-46}$$

and the two orthonormalization relations:

$$\langle u_i | u_j \rangle = \delta_{ij} \tag{C-47}$$

$$\langle t_k | t_l \rangle = \delta_{kl} \tag{C-48}$$

COMMENT:

The transformation matrix, S, is unitary (complement C_{II}). That is, it satisfies:

$$S^\dagger S = SS^\dagger = I \tag{C-49}$$

where I is the unit matrix. Indeed, we see that:

$$(S^\dagger S)_{kl} = \sum_i S^\dagger_{ki} S_{il} = \sum_i \langle t_k | u_i \rangle \langle u_i | t_l \rangle = \langle t_k | t_l \rangle = \delta_{kl} \tag{C-50}$$

In the same way:

$$(SS^\dagger)_{ij} = \sum_k S_{ik} S^\dagger_{kj} = \sum_k \langle u_i | t_k \rangle \langle t_k | u_j \rangle = \langle u_i | u_j \rangle = \delta_{ij} \tag{C-51}$$

b. TRANSFORMATION OF THE COMPONENTS OF A KET

To obtain the components $\langle t_k | \psi \rangle$ of a ket $|\psi\rangle$ in the new basis from its components $\langle u_i | \psi \rangle$ in the old basis, one simply inserts (C-45) between $\langle t_k |$ and $|\psi\rangle$:

$$\langle t_k | \psi \rangle = \langle t_k | \mathbb{1} | \psi \rangle = \langle t_k | P_{\{u_i\}} | \psi \rangle = \sum_i \langle t_k | u_i \rangle \langle u_i | \psi \rangle = \sum_i S^\dagger_{ki} \langle u_i | \psi \rangle \tag{C-52}$$

The inverse expressions can be derived in the same way, using (C-46):

$$\langle u_i | \psi \rangle = \langle u_i | \mathbb{1} | \psi \rangle = \langle u_i | P_{\{t_k\}} | \psi \rangle = \sum_k \langle u_i | t_k \rangle \langle t_k | \psi \rangle = \sum_k S_{ik} \langle t_k | \psi \rangle \tag{C-53}$$

c. TRANSFORMATION OF THE COMPONENTS OF A BRA

The principle of the calculation is exactly the same. For example:

$$\langle \psi | t_k \rangle = \langle \psi | \mathbb{1} | t_k \rangle = \langle \psi | P_{\{u_i\}} | t_k \rangle = \sum_i \langle \psi | u_i \rangle \langle u_i | t_k \rangle = \sum_i \langle \psi | u_i \rangle S_{ik} \tag{C-54}$$

d. TRANSFORMATION OF THE MATRIX ELEMENTS OF AN OPERATOR

If, in $\langle t_k | A | t_l \rangle$, we insert (C-45) between $\langle t_k |$ and A, and again between A and $|t_l\rangle$, we obtain:

$$\langle t_k | A | t_l \rangle = \langle t_k | P_{\{u_i\}} A \; P_{\{u_j\}} | t_l \rangle = \sum_{i,j} \langle t_k | u_i \rangle \langle u_i | A | u_j \rangle \langle u_j | t_l \rangle \tag{C-55}$$

that is:

$$A_{kl} = \sum_{i,j} S^\dagger_{ki} \; A_{ij} \; S_{jl} \tag{C-56}$$

In the same way:

$$A_{ij} = \langle u_i | A | u_j \rangle = \langle u_i | P_{\{t_k\}} A \; P_{\{t_l\}} | u_j \rangle = \sum_{k,l} \langle u_i | t_k \rangle \langle t_k | A | t_l \rangle \langle t_l | u_j \rangle = \sum_{k,l} S_{ik} \; A_{kl} \; S^\dagger_{lj} \tag{C-57}$$

D. EIGENVALUE EQUATIONS. OBSERVABLES

1. Eigenvalues and eigenvectors of an operator

a. DEFINITIONS

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

$$\boxed{A|\psi\rangle = \lambda|\psi\rangle} \tag{D-1}$$

where λ is a complex number. We are going to study a certain number of properties of equation (D-1), *the eigenvalue equation of the linear operator A*. In general, this equation possesses solutions only when λ takes on certain values, called *eigenvalues* of A. The set of the eigenvalues is called the *spectrum* of A.

Note that, if $|\psi\rangle$ is an eigenvector of A with the eigenvalue λ, $\alpha|\psi\rangle$ (where α is an arbitrary complex number) is also an eigenvector of A with the same eigenvalue:

$$A(\alpha|\psi\rangle) = \alpha A|\psi\rangle = \alpha\lambda|\psi\rangle = \lambda(\alpha|\psi\rangle) \tag{D-2}$$

To rid ourselves of this ambiguity, we could agree to normalize the eigenvectors to 1:

$$\langle\psi|\psi\rangle = 1 \tag{D-3}$$

But this does not completely remove the ambiguity, since $e^{i\theta}|\psi\rangle$, where θ is an arbitrary real number, has the same norm as $|\psi\rangle$. We shall see below that, in quantum mechanics, the physical predictions obtained using $|\psi\rangle$ or $e^{i\theta}|\psi\rangle$ are the same.

The eigenvalue λ is called *nondegenerate* (or *simple*) when its corresponding eigenvector is unique to within a constant factor, that is, when all its associated eigenkets are collinear. On the other hand, if there exist at least two linearly independent kets which are eigenvectors of A with the same eigenvalue, this eigenvalue is said to be *degenerate*. Its *degree* (or *order*) *of degeneracy* is then the number of linearly independent eigenvectors which are associated with it (the degree of degeneracy of an eigenvalue can be finite or infinite). For example, if λ is g-fold degenerate, there correspond to it g independent kets $|\psi^i\rangle$ $(i = 1, 2, \ldots g)$ such that:

$$A|\psi^i\rangle = \lambda|\psi^i\rangle \tag{D-4}$$

But then every ket $|\psi\rangle$ of the form:

$$|\psi\rangle = \sum_{i=1}^{g} c_i|\psi^i\rangle \tag{D-5}$$

is an eigenvector of A with the eigenvalue λ, whatever the coefficients c_i, since:

$$A|\psi\rangle = \sum_{i=1}^{g} c_i A|\psi^i\rangle = \lambda\sum_{i=1}^{g} c_i|\psi^i\rangle = \lambda|\psi\rangle \tag{D-6}$$

Consequently, the set of eigenkets of A associated with λ constitutes a *g-dimensional vector space* (which can be infinite-dimensional), called the "*eigensubspace*" of the eigenvalue λ. In particular, it is equivalent to say that λ is non-degenerate or to say that its degree of degeneracy is $g = 1$.

To illustrate these definitions, let us choose the example of a projector (§ B-3-b): $P_\psi = |\psi\rangle\langle\psi|$ (with $\langle\psi|\psi\rangle = 1$). Its eigenvalue equation is written:

$$P_\psi|\varphi\rangle = \lambda|\varphi\rangle$$

that is,

$$|\psi\rangle\langle\psi|\varphi\rangle = \lambda|\varphi\rangle \tag{D-7}$$

The ket on the left-hand side is always collinear with $|\psi\rangle$ or zero. Consequently, the eigenvectors of P_ψ are: on the one hand, $|\psi\rangle$ itself, with an eigenvalue of $\lambda = 1$; on the other hand, all the kets $|\varphi\rangle$ orthogonal to $|\psi\rangle$, for which the associated eigenvalue is $\lambda = 0$. The spectrum of P_ψ therefore includes only two values: 1 and 0. The first one is simple, the second, infinitely degenerate (if the state space considered is infinite-dimensional). The eigensubspace associated with $\lambda = 0$ is the supplement* of $|\psi\rangle$ (see §D-2-c).

COMMENTS:

(*i*) Taking the Hermitian conjugate of both sides of equation (D-1), we obtain:

$$\langle\psi|A^\dagger = \lambda^*\langle\psi| \tag{D-8}$$

Therefore, if $|\psi\rangle$ is an eigenket of A with an eigenvalue λ, it can also be said that $\langle\psi|$ is an eigenbra of $A^\dagger$ with an eigenvalue λ^*. However, let us stress the fact that, except in the case where A is Hermitian (§ D-2-a), nothing can be said *a priori* about $\langle\psi|A$.

(*ii*) To be completely rigorous, one should solve the eigenvalue equation (D-1) in the space $\mathcal{E}$. That is, one should consider only those eigenvectors $|\psi\rangle$ which have a finite norm. In fact, we shall be obliged to use operators for which the eigenkets do not satisfy this condition (§ E). Therefore, we shall grant that vectors which are solutions of (D-1) can be "generalized kets".

b. FINDING THE EIGENVALUES AND EIGENVECTORS OF AN OPERATOR

Given a linear operator A, how does one find all its eigenvalues and the corresponding eigenvectors? We are concerned with this question from a purely practical point of view. We shall consider the case where the state space is of finite dimension N, and we shall grant that the results can be generalized to an infinite-dimensional state space.

Let us choose a representation, for example, $\{|u_i\rangle\}$, and let us project the vector equation (D-1) onto the various orthonormal basis vectors $|u_i\rangle$:

$$\langle u_i|A|\psi\rangle = \lambda\langle u_i|\psi\rangle \tag{D-9}$$

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

$$\sum_j \langle u_i|A|u_j\rangle\langle u_j|\psi\rangle = \lambda\langle u_i|\psi\rangle \tag{D-10}$$

* In a vector space $\mathcal{E}$, two sub-spaces $\mathcal{E}_1$ and $\mathcal{E}_2$ are said to be supplementary if all kets $|\psi\rangle$ of $\mathcal{E}$ can be written $|\psi\rangle = |\psi_1\rangle + |\psi_2\rangle$ where $|\psi_1\rangle$ and $|\psi_2\rangle$ belong, respectively, to $\mathcal{E}_1$ and $\mathcal{E}_2$, and if $\mathcal{E}_1$ and $\mathcal{E}_2$ are disjoint (no common non-zero ket; the expansion $|\psi\rangle = |\psi_1\rangle + |\psi_2\rangle$ is then unique). Actually, there exists an infinity of sub-subspaces $\mathcal{E}_2$ supplementary to a given sub-space $\mathcal{E}_1$. One can fix $\mathcal{E}_2$ by forcing it to be orthogonal to $\mathcal{E}_1$. This shall be done throughout this book, even though the word "orthogonal" will not be explicitly written before supplement.

Example: In ordinary three-dimensional space, if $\mathcal{E}_1$ is a plane P, $\mathcal{E}_2$ can be any arbitrary straight line, not contained in P. The orthogonal supplement of $\mathcal{E}_1$ is the straight line passing through the origin and orthogonal to P.

With the usual notation :

$$\langle u_i \mid \psi \rangle = c_i$$
$$\langle u_i \mid A \mid u_j \rangle = A_{ij} \tag{D-11}$$

equations (D-10) can be written:

$$\sum_j A_{ij}\ c_j = \lambda c_i \tag{D-12}$$

or

$$\sum_j [A_{ij} - \lambda\delta_{ij}]c_j = 0 \tag{D-13}$$

(D-13) can be considered to be a system of equations where the unknowns are the c_j, the components of the eigenvector in the chosen representation. This system is linear and homogeneous.

α. *The characteristic equation*

The system (D-13) consists of N equations ($i = 1, 2, ..., N$) in N unknowns c_j ($j = 1, 2, ..., N$). Since it is linear and homogeneous, it has a non-trivial solution (the trivial solution is the one for which all the c_j are zero) if and only if the determinant of the coefficients is zero. This condition is written:

$$\boxed{\text{Det}\,[\mathscr{A} - \lambda I] = 0} \tag{D-14}$$

where $\mathscr{A}$ is the $N \times N$ matrix of elements A_{ij} and I is the unit matrix.

Equation (D-14), called the characteristic equation (or secular equation), enables us to determine all the eigenvalues of the operator A, that is, its spectrum. (D-14) can be written explicitly in the form:

$$\begin{vmatrix} A_{11} - \lambda & A_{12} & A_{13} \ldots & A_{1N} \\ A_{21} & A_{22} - \lambda & A_{23} \ldots & A_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ A_{N1} & A_{N2} & A_{N3} \ldots & A_{NN} - \lambda \end{vmatrix} = 0 \tag{D.15}$$

This is an Nth order equation in λ; consequently, it has N roots, real or imaginary, distinct or identical. It is easy to show, by performing an arbitrary change of basis, that the characteristic equation is independent of the representation chosen. Therefore, *the eigenvalues of an operator are the roots of its characteristic equation.*

β. *Determination of the eigenvectors*

Now let us choose an eigenvalue λ_0, a solution of the characteristic equation (D-14), and let us look for the corresponding eigenvectors. We are going to distinguish between two cases:

(*i*) First, assume that λ_0 is a simple root of the characteristic equation. We can then show that the system (D-13), when $\lambda = \lambda_0$, is comprised of $(N - 1)$ independent equations, the Nth one following from the preceding ones and hence

redundant. But we have N unknowns; there is therefore an infinite number of solutions, but all the c_j can be determined in a unique way in terms of one of them, say c_1. If we fix c_1, we obtain for the $(N - 1)$ other c_j a system of $(N - 1)$ linear, inhomogeneous equations (the "right-hand side" of each equation is the term in c_1) with a non-zero determinant [the $(N - 1)$ equations are independent]. The solution of this system is of the form:

$$c_j = \alpha_j^0\ c_1 \tag{D-16}$$

since the initial system (D-13) is linear and homogeneous. α_1^0 is, of course, equal to 1 by definition, and the $(N - 1)$ coefficients α_j^0 for $j \neq 1$ 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:

$$|\, \psi_0(c_1) \rangle = \sum_j \alpha_j^0\ c_1 |\, u_j \rangle = c_1 \mid \psi_0 \rangle \tag{D-17}$$

with:

$$|\, \psi_0 \rangle = \sum_j \alpha_j^0 \mid u_j \rangle \tag{D-18}$$

Therefore, when λ_0 is a simple root of the characteristic equation, only one eigenvector corresponds to it (to within a constant factor): it is a non-degenerate eigenvalue.

(*ii*) When λ_0 is a multiple root of order $q > 1$ of the characteristic equation, there are two possibilities:

– in general, when $\lambda = \lambda_0$, the system (D-13) is still composed of $(N - 1)$ independent equations. Only one eigenvector then corresponds to the eigenvalue λ_0. The operator A cannot be diagonalized in this case : the eigenvectors of A are not sufficiently numerous for one to be able to construct with them alone a basis of the state space.

– nevertheless, when $\lambda = \lambda_0$, it may happen that the system (D-13) has only $(N - p)$ independent equations (where p is a number greater than 1 but not larger than q). To the eigenvalue λ_0 there then corresponds an eigensubspace of dimension p, and λ_0 is a p-fold degenerate eigenvalue. Let us assume, for example, that, for $\lambda = \lambda_0$, (D-13) is composed of $(N - 2)$ linearly independent equations. These equations enable us to calculate the coefficients c_j in terms of any two of them, for example c_1 and c_2:

$$c_j = \beta_j^0 c_1 + \gamma_j^0 c_2 \tag{D-19}$$

(obviously : $\beta_1^0 = \gamma_2^0 = 1$; $\gamma_1^0 = \beta_2^0 = 0$). All the eigenvectors associated with λ_0 are then of the form:

$$|\, \psi_0(c_1, c_2) \rangle = c_1 \mid \psi_0^1 \rangle + c_2 \mid \psi_0^2 \rangle \tag{D-20}$$

with:

$$|\, \psi_0^1 \rangle = \sum_j \beta_j^0 \mid u_j \rangle$$

$$|\psi_0^2\rangle = \sum_j \gamma_j^0 |u_j\rangle \tag{D-21}$$

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

When an operator is Hermitian, it can be shown that the degree of degeneracy p of an eigenvalue λ is always equal to the multiplicity q of the corresponding root in the characteristic equation. Since, in most cases, we shall be studying only Hermitian operators, we shall only need to know the multiplicity of each root of (D-14) to obtain immediately the dimension of the corresponding eigensubspace. Thus, in a space of finite dimension N, a Hermitian operator always has N linearly independent eigenvectors (we shall see later that they can be chosen to be orthonormal): this operator can therefore be diagonalized (§ D-2-b).

2. Observables

a. PROPERTIES OF THE EIGENVALUES AND EIGENVECTORS OF A HERMITIAN OPERATOR

We shall now consider the very important case in which the operator A is Hermitian:

$$A^\dagger = A \tag{D-22}$$

(*i*) *The eigenvalues of a Hermitian operator are real*

Taking the scalar product of the eigenvalue equation (D-1) by $|\psi\rangle$, we obtain:

$$\langle\psi|A|\psi\rangle = \lambda\langle\psi|\psi\rangle \tag{D-23}$$

But $\langle\psi|A|\psi\rangle$ is a real number if A is Hermitian, as we see from:

$$\langle\psi|A|\psi\rangle^* = \langle\psi|A^\dagger|\psi\rangle = \langle\psi|A|\psi\rangle \tag{D-24}$$

where the last equation follows from hypothesis (D-22). Since $\langle\psi|A|\psi\rangle$ and $\langle\psi|\psi\rangle$ are real, equation (D-23) implies that λ must also be real.

If A is Hermitian, we can, in (D-8), replace A by $A^\dagger$ and λ by λ^*, since we have just shown that λ is real. Thus we obtain:

$$\langle\psi|A = \lambda\langle\psi| \tag{D-25}$$

which shows that $\langle\psi|$ is also an eigenbra of A with the real eigenvalue λ. Therefore, whatever the ket $|\varphi\rangle$:

$$\langle\psi|A|\varphi\rangle = \lambda\langle\psi|\varphi\rangle \tag{D-26}$$

The Hermitian operator A is said to act on the left in (D-26).

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

Consider two eigenvectors $|\psi\rangle$ and $|\varphi\rangle$ of the Hermitian operator A:

$$A|\psi\rangle = \lambda|\psi\rangle \tag{D-27-a}$$
$$A|\varphi\rangle = \mu|\varphi\rangle \tag{D-27-b}$$

Since A is Hermitian, (D-27-b) can be written in the form:

$$\langle\varphi|A = \mu\langle\varphi| \tag{D-28}$$

Then multiply (D-27-a) by $\langle\varphi|$ on the left and (D-28) by $|\psi\rangle$ on the right:

$$\langle\varphi|A|\psi\rangle = \lambda\langle\varphi|\psi\rangle \tag{D-29-a}$$
$$\langle\varphi|A|\psi\rangle = \mu\langle\varphi|\psi\rangle \tag{D-29-b}$$

Subtracting (D-29-b) from (D-29-a), we find:

$$(\lambda - \mu)\langle\varphi|\psi\rangle = 0 \tag{D-30}$$

Consequently, if $(\lambda - \mu) \neq 0$, $|\varphi\rangle$ and $|\psi\rangle$ are orthogonal.

b. DEFINITION OF AN OBSERVABLE

When $\mathscr{E}$ is finite-dimensional, we have seen (§ D-1-b) that it is always possibl to form a basis with the eigenvectors of a Hermitian operator. When $\mathscr{E}$ is infinite dimensional, this is no longer necessarily the case. This is why it is useful to introduc a new concept, that of an observable.

Consider a Hermitian operator A. For simplicity, we shall assume that th set of its eigenvalues forms a discrete spectrum $\{a_n; n = 1, 2, \ldots\}$, and we sha indicate later the modifications that must be made when all or part of this spectrur is continuous. The degree of degeneracy of the eigenvalue a_n will be denote by g_n (if $g_n = 1$, a_n is non-degenerate). We shall denote by $|\psi_n^i\rangle$ ($i = 1, 2, \ldots, g_n$ g_n linearly independent vectors chosen in the eigensubspace $\mathscr{E}_n$ of a_n:

$$A|\psi_n^i\rangle = a_n|\psi_n^i\rangle; \quad i = 1, 2, \ldots, g_n \tag{D-31}$$

We have just shown that every vector belonging to $\mathscr{E}_n$ is orthogonal to ever vector of another subspace $\mathscr{E}_{n'}$, associated with $a_{n'} \neq a_n$; therefore:

$$\langle\psi_n^i|\psi_{n'}^j\rangle = 0 \quad \text{for } n \neq n' \text{ and arbitrary } i \text{ and } j \tag{D-32}$$

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

$$\langle\psi_n^i|\psi_n^j\rangle = \delta_{ij} \tag{D-33}$$

If such a choice is made, the result is an *orthonormal system of eigenvector of* A: the $|\psi_n^i\rangle$ satisfy the relations:

$$\boxed{\langle\psi_n^i|\psi_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'}} \tag{D-34}$$

obtained by regrouping (D-32) and (D-33).

By definition, the Hermitian operator A is an *observable* if this orthonorma system of vectors *forms a basis* in the state space. This can be expressed by th closure relation:

$$\boxed{\sum_{n=1}^{\infty}\sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i| = \mathbb{1}} \tag{D-35}$$

COMMENTS:

(*i*) Since the g_n vectors $|\psi_n^i\rangle$ ($i = 1, 2, \ldots, g_n$) which span the eigensubspace $\mathcal{E}_n$ of a_n are orthonormal, the projector P_n onto this subspace $\mathcal{E}_n$ can be written (*cf.* § B-3-b-γ):

$$P_n = \sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i| \tag{D-36-a}$$

The observable A is then given by:

$$A = \sum_n a_n P_n \tag{D-36-b}$$

(it is easy to verify that the action of both sides of this equation on all the kets $|\psi_n^i\rangle$ gives the same result).

(*ii*) Relation (D-35) can be generalized to include cases where the spectrum of eigenvalues is continuous by using the rules given in table (II-3). For example, consider a Hermitian operator whose spectrum is composed of a discrete part $\{ a_n$ (degree of degeneracy $g_n) \}$ and a continuous part $a(v)$ (assumed to be non-degenerate):

$$A|\psi_n^i\rangle = a_n|\psi_n^i\rangle; \quad \begin{matrix} n = 1, 2, \ldots \\ i = 1, 2, \ldots g_n \end{matrix} \tag{D-37-a}$$

$$A|\psi_v\rangle = a(v)|\psi_v\rangle; \quad v_1 < v < v_2 \tag{D-37-b}$$

These vectors can always be chosen in such a way that they form an "orthonormal" system:

$$\begin{aligned} &\langle\psi_n^i|\psi_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'} \\ &\langle\psi_v|\psi_{v'}\rangle = \delta(v - v') \\ &\langle\psi_n^i|\psi_v\rangle = 0 \end{aligned} \tag{D-38}$$

A will be said to be an observable if this system forms a basis, that is, if:

$$\sum_n \sum_{i=1}^{g_n} |\psi_n^i\rangle\langle\psi_n^i| + \int_{v_1}^{v_2} dv\, |\psi_v\rangle\langle\psi_v| = \mathbb{1} \tag{D-39}$$

c. EXAMPLE: THE PROJECTOR P_ψ

Let us show that $P_\psi = |\psi\rangle\langle\psi|$ (with $\langle\psi|\psi\rangle = 1$) is an observable. We have already pointed out (§ B-4-e) that it is Hermitian, and that its eigenvalues are 1 and 0 (§ D-1-a); the first one is simple (associated eigenvector: $|\psi\rangle$), the second one is infinitely degenerate (associated eigenvectors: all kets orthogonal to $|\psi\rangle$).

Consider an arbitrary ket $|\varphi\rangle$ in the state space. It can always be written in the form:

$$|\varphi\rangle = P_\psi|\varphi\rangle + (\mathbb{1} - P_\psi)|\varphi\rangle \tag{D-40}$$

$P_\psi|\varphi\rangle$ is an eigenket of P_ψ with the eigenvalue 1. Now, since $P_\psi^2 = P_\psi$:

$$P_\psi(P_\psi|\varphi\rangle) = P_\psi^2|\varphi\rangle = P_\psi|\varphi\rangle \tag{(}$$

$(\mathbb{1} - P_\psi)|\varphi\rangle$ is also an eigenket of P_ψ, but with the eigenvalue 0, as we see f

$$P_\psi(\mathbb{1} - P_\psi)|\varphi\rangle = (P_\psi - P_\psi^2)|\varphi\rangle = 0. \tag{(}$$

Every ket $|\varphi\rangle$ can thus be expanded on these eigenkets of P_ψ; ther P_ψ is an observable.

We shall see in § E-2 two other important examples of observables.

3. Sets of commuting observables

a. IMPORTANT THEOREMS

α. *Theorem I*

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

We know that, if $|\psi\rangle$ is an eigenvector of A, we have:

$$A|\psi\rangle = a|\psi\rangle \tag{I}$$

Applying B to both sides of this equation, we obtain:

$$BA|\psi\rangle = aB|\psi\rangle \tag{I}$$

Since we assumed that A and B commute, we also have, replacing BA on the left-side by AB:

$$A(B|\psi\rangle) = a(B|\psi\rangle) \tag{I}$$

This equation expresses the fact that $B|\psi\rangle$ is an eigenvector of A, with the e value a; the theorem is therefore proved.

Two cases may then arise:

(*i*) If a is a nondegenerate eigenvalue, all the eigenvectors associated it are by definition colinear, and $B|\psi\rangle$ is necessarily proportional to Therefore $|\psi\rangle$ is also an eigenvector of B.

(*ii*) If a is a degenerate eigenvalue, it can only be said that $B|\psi\rangle$ bel to the eigensubspace $\mathcal{E}_a$ of A, corresponding to the eigenvalue a. There for any $|\psi\rangle \in \mathcal{E}_a$, we have:

$$B|\psi\rangle \in \mathcal{E}_a \tag{I}$$

$\mathcal{E}_a$ is said to be globally invariant (or stable) under the action of B. Theorem I therefore be stated in another form:

Theorem I': If two operators A and B commute, every eigensubspace is globally invariant under the action of B.

β. *Theorem II*

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

If $|\psi_1\rangle$ and $|\psi_2\rangle$ are eigenvectors of A, we can write:

$$A|\psi_1\rangle = a_1|\psi_1\rangle$$
$$A|\psi_2\rangle = a_2|\psi_2\rangle \qquad \text{(D-47)}$$

According to theorem I, the fact that A and B commute means that $B|\psi_2\rangle$ is an eigenvector of A, with the eigenvalue a_2. $B|\psi_2\rangle$ is therefore (*cf.* § D-2-a) orthogonal to $|\psi_1\rangle$ (eigenvector of eigenvalue $a_1 \neq a_2$), which can be written:

$$\langle\psi_1|B|\psi_2\rangle = 0 \qquad \text{(D-48)}$$

The theorem is therefore proved. Another proof can be given, which does not involve theorem I: since the operator $[A, B]$ is zero, we have:

$$\langle\psi_1|(AB - BA)|\psi_2\rangle = 0 \qquad \text{(D-49)}$$

Using (D-47) and the Hermiticity of A [*cf.* equation (D-25)], we obtain:

$$\langle\psi_1|AB|\psi_2\rangle = a_1\langle\psi_1|B|\psi_2\rangle$$
$$\langle\psi_1|BA|\psi_2\rangle = a_2\langle\psi_1|B|\psi_2\rangle \qquad \text{(D-50)}$$

and (D-49) can be rewritten in the form:

$$(a_1 - a_2)\langle\psi_1|B|\psi_2\rangle = 0 \qquad \text{(D-51)}$$

Since, by hypothesis, $(a_1 - a_2)$ is not zero, we can deduce (D-48) from this.

γ. *Theorem III (fundamental)*

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

Consider two commuting observables, A and B. In order to simplify the notation, we shall assume that their spectra are entirely discrete. Since A is an observable, there exists at least one orthonormal system of eigenvectors of A which forms a basis in the state space. We shall denote these vectors by $|u_n^i\rangle$:

$$A|u_n^i\rangle = a_n|u_n^i\rangle; \quad n = 1, 2, \ldots \quad i = 1, 2, \ldots, g_n \qquad \text{(D-52)}$$

g_n is the degree of degeneracy of the eigenvalue a_n, that is, the dimension of the corresponding eigensubspace $\mathscr{E}_n$. We have:

$$\langle u_n^i|u_{n'}^{i'}\rangle = \delta_{nn'}\delta_{ii'} \qquad \text{(D-53)}$$

What does the matrix look like which represents B in the $\{|u_n^i\rangle\}$ basis? We know (*cf.* theorem II) that the matrix elements $\langle u_n^i|B|u_{n'}^{i'}\rangle$ are zero when $n \neq n'$ (on the other hand, we can say nothing *a priori* about what happens for $n = n'$ and $i \neq i'$). Let us arrange the basis vectors $|u_n^i\rangle$ in the order :

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

We then obtain for B a "block-diagonal" matrix, that is, of the form:

	$\mathscr{E}_1$	$\mathscr{E}_2$	$\mathscr{E}_3$	...
$\mathscr{E}_1$		0	0	0
$\mathscr{E}_2$	0		0	0
$\mathscr{E}_3$	0	0		0
⋮	0	0	0	

(D

(only the shaded parts contain non-zero matrix elements). The fact that eigensubspaces $\mathscr{E}_n$ are globally invariant under the action of B (*cf.* § α) is evic from this matrix.

Two cases can then arise:

(*i*) When a_n is a nondegenerate eigenvalue of A, there exists only one eig vector $|u_n\rangle$ of A, of eigenvalue a_n (the index i in $|u_n\rangle$ is then unnecessary): dimension g_n of $\mathscr{E}_n$ is then equal to 1. In the matrix (D-54), the corresponding "blo then reduces to a 1×1 matrix, that is, to a simple number. In the column associa with $|u_n\rangle$, all the other matrix elements are zero. This expresses the fact (*cf.* § that $|u_n\rangle$ is an eigenvector common to A and B.

(*ii*) When a_n is a degenerate eigenvalue of A ($g_n > 1$), the "block" wh represents B in $\mathscr{E}_n$ is not, in general, diagonal : the $|u_n^i\rangle$ are not, in general, eig vectors of B.

It can be seen, nevertheless, that, since the action of A on each of the vectors $|u_n^i\rangle$ reduces to a simple multiplication by a_n, the matrix represen the restriction of A to within $\mathscr{E}_n$ is equal to $a_n I$ (where I is the $g_n \times g_n$ unit mat This expresses the fact that an arbitrary ket of $\mathscr{E}_n$ is an eigenvector of A with eigenvalue a_n. The choice, in $\mathscr{E}_n$ of a basis such as $\{|u_n^i\rangle; i = 1, 2, \ldots, g_n$ therefore arbitrary. Whatever this basis, the matrix representing A in $\mathscr{E}_n$ is alw diagonal and equal to $a_n I$. We shall use this property to obtain a basis of $\mathscr{E}_n$ compo of vectors which are also eigenvectors of B.

The matrix representing B in $\mathscr{E}_n$, when the basis chosen is

$$\{|u_n^i\rangle; i = 1, 2, \ldots, g_n\},$$

has for its elements:

$$\beta_{ij}^{(n)} = \langle u_n^i|B|u_n^j\rangle \qquad \text{(D-}$$

This matrix is Hermitian ($\beta_{ji}^{(n)*} = \beta_{ij}^{(n)}$), since B is a Hermitian operator. It is theref diagonalizable, that is, *one can find in* $\mathscr{E}_n$ *a new basis* $\{|v_n^i\rangle; i = 1, 2, \ldots, g_n\}$ *which B is represented by a diagonal matrix*

$$\langle v_n^i|B|v_n^j\rangle = \beta_i^{(n)}\delta_{ij} \qquad \text{(D-}$$

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

$$B|v_n^i\rangle = \beta_i^{(n)}|v_n^i\rangle \tag{D-57}$$

As we saw above, these vectors are automatically eigenvectors of A with an eigenvalue a_n since they belong to $\mathcal{E}_n$. Let us stress the fact that *the eigenvectors of A associated with degenerate eigenvalues are not necessarily eigenvectors of B.* What we have just shown is that *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 subspaces $\mathcal{E}_n$, we obtain a basis of $\mathcal{E}$, formed by eigenvectors common to A and B. The theorem is therefore proved.

COMMENTS:

(*i*) From now on, we shall denote by $|u_{n,p}^i\rangle$ the eigenvectors common to A and B.

$$\begin{aligned} A|u_{n,p}^i\rangle &= a_n|u_{n,p}^i\rangle \\ B|u_{n,p}^i\rangle &= b_p|u_{n,p}^i\rangle \end{aligned} \tag{D-58}$$

The indices n and p which appear in $|u_{n,p}^i\rangle$ enable us to specify the eigenvalues a_n and b_p of A and B. The additional index i will eventually be used to distinguish between the different basis vectors which correspond to the same eigenvalues a_n and b_p (§ b below).

(*ii*) The converse of theorem III is very simple to prove: if there exists a basis of eigenvectors common to A and B, these two observables commute. From (D-58), it is easy to deduce:

$$\begin{aligned} AB|u_{n,p}^i\rangle &= b_p A|u_{n,p}^i\rangle = b_p a_n|u_{n,p}^i\rangle \\ BA|u_{n,p}^i\rangle &= a_n B|u_{n,p}^i\rangle = a_n b_p|u_{n,p}^i\rangle \end{aligned} \tag{D-59}$$

and, subtracting these equations:

$$[A, B]|u_{n,p}^i\rangle = 0 \tag{D-60}$$

This relation is valid for all i, n and p. Since, by hypothesis, the vectors $|u_{n,p}^i\rangle$ form a basis, (D-60) entails $[A, B] = 0$.

(*iii*) We shall occasionally solve the eigenvalue equation of an observable C such that:

$$C = A + B \quad \text{with} \quad [A, B] = 0 \tag{D-61}$$

where A and B are also observables.

When one has found a basis $\{|u_{n,p}^i\rangle\}$ of eigenvectors common to A and B, the problem is solved, since we see immediately that $|u_{n,p}^i\rangle$ is also an eigenvector of C, with an eigenvalue $a_n + b_p$. The fact that $\{|u_{n,p}^i\rangle\}$ constitutes a basis is obviously essential: this allows us, for example, to show simply that all the eigenvalues of C are of the form $a_n + b_p$.

b. COMPLETE* SETS OF COMMUTING OBSERVABLES (C.S.C.O.)**

Consider an observable A and a basis of $\mathcal{E}$ composed of eigenvectors $|u$ of A. If none of the eigenvalues of A is degenerate, the various basis vectors of can be labelled by the eigenvalue a_n (the index i in $|u_n^i\rangle$ being in this case unnec sary). All the eigensubspaces $\mathcal{E}_n$ are then one-dimensional. Therefore, specifyi the eigenvalue determines in a unique way the corresponding eigenvector within a constant factor). In other words, there exists only one basis of $\mathcal{E}$ form by the eigenvectors of A (we shall not consider here as distinct two bases whc vectors are proportional). It is then said that the observable A constitutes, itself, a C.S.C.O.

If, on the other hand, one or several eigenvalues of A are degenerate, t situation is different. Specifying a_n is no longer always sufficient to characteri a basis vector, since there correspond several independent vectors to degenerate eige values. In this case, the basis of eigenvectors of A is obviously not unique. One c choose any basis inside each of the eigensubspaces $\mathcal{E}_n$ of dimension greater than

Let us then choose another observable B which commutes with A, and let construct an orthonormal basis of eigenvectors common to A and B. By definitic A and B form a C.S.C.O. if this basis is unique (to within a phase factor for each the basis vectors), that is, if, to each of the possible pairs of eigenvalues $\{a_n, b_p$ there corresponds only one basis vector.

COMMENT:

In § a, we constructed a basis of eigenvectors common to A and B by solv the eigenvalue equation of B inside each eigensubspace $\mathcal{E}_n$. For A and B to constitu a C.S.C.O., it is necessary and sufficient that, inside each of these subspaces, all the eigenvalues of B be distinct. Since all the vectors of $\mathcal{E}_n$ correspond to the sa eigenvalue a_n of A, the g_n vectors $|v_n^i\rangle$ can then be distinguished by the eigenva of B which is associated with them. Note that it is not necessary that all the eigenvalues o be non-degenerate. Vectors $|v_n^i\rangle$ belonging to two distinct subspaces $\mathcal{E}_n$ can have same eigenvalue for B. Moreover, if all the eigenvalues of B were non-degenerate, B alc would constitute a C.S.C.O.

If, for at least one of the possible pairs $\{a_n, b_p\}$, there exist seve independent vectors which are eigenvectors of A and B with these eigenvalu the set $\{A, B\}$ is not complete. Let us add to it, then, a third observable which commutes with both A and B. We can then use the same argume as in § a above, generalizing it in the following way. When to a pair $\{a_n, b_p$ there corresponds only one vector, this vector is necessarily an eigenvector of If there are several vectors, they form an eigensubspace $\mathcal{E}_{n,p}$, in which it is possil to choose a basis formed by vectors which are also eigenvectors of C. One c thus construct, in the state space, an orthonormal basis formed by eigenvectc common to A, B and C. A, B and C form a C.S.C.O. if this basis is uniq

* The word "complete" is used here in a sense which is totally unrelated to those referred tc the note of § A-2-a, p. 97. This use of the word "complete" is customary in quantum mechanics.

** To have a good understanding of the important concepts introduced in this section, reader should apply them to a concrete example such as the one discussed in complement H_{II} (sol exercises 11 and 12).

(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 $| a_n, b_p, c_r, \ldots \rangle$.

(*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 $\mathscr{E}_\mathbf{r}$ 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 $\mathscr{E}_\mathbf{r}$; this correspondence is linear. Moreover, the scalar product of two kets coincides with that of the functions which are associated with them:

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

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

We are going to define and study, in this space, two representations two operators which are particularly important. In chapter III we shall assoc them with the position and the momentum of the particle under considerat They will enable us, moreover, to apply and illustrate the concepts which we h 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 $\mathscr{E}$ $\{ \xi_{\mathbf{r}_0}(\mathbf{r}) \}$ and $\{ v_{\mathbf{p}_0}(\mathbf{r}) \}$. They are not composed of functions belonging to $\mathscr{E}$

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

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

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

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

$$\boxed{\begin{array}{l} \xi_{\mathbf{r}_0}(\mathbf{r}) \iff | \mathbf{r}_0 \rangle \\ v_{\mathbf{p}_0}(\mathbf{r}) \iff | \mathbf{p}_0 \rangle \end{array}} \qquad \begin{array}{l} \text{(E-} \\ \text{(E-} \end{array}$$

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

b. ORTHONORMALIZATION AND CLOSURE RELATIONS

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

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

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

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