Complement B_{II}

REVIEW OF SOME USEFUL PROPERTIES OF LINEAR OPERATORS

The aim of this complement is to review a certain number of definitions and useful properties of linear operators.

1. Trace of an operator

a. DEFINITION

The trace of an operator A, written Tr A, is the sum of its diagonal matrix elements.

When a discrete orthonormal basis, $\{ | u_i \rangle \}$, is chosen for the space $\mathscr{E}$, one has, by definition:

$$\text{Tr}\, A = \sum_i \langle u_i | A | u_i \rangle \tag{1}$$

For the case of a continuous orthonormal basis $\{ | w_\alpha \rangle \}$, one has:

$$\text{Tr}\, A = \int d\alpha \, \langle w_\alpha | A | w_\alpha \rangle \tag{2}$$

When $\mathscr{E}$ is an infinite-dimensional space, the trace of the operator A is defined only if expressions (1) and (2) converge.

b. THE TRACE IS INVARIANT

The sum of the diagonal elements of the matrix which represents an operator A in an arbitrary basis does not depend on this basis.

Let us derive this property for the case of a change from one discrete orthonormal basis $\{ | u_i \rangle \}$ to another discrete orthonormal basis $\{ | t_k \rangle \}$. We have:

$$\sum_i \langle u_i | A | u_i \rangle = \sum_i \langle u_i | \left[\sum_k | t_k \rangle \langle t_k | \right] A | u_i \rangle \tag{3}$$

(where we have used the closure relation for the $| t_k \rangle$ states). The right-hand side of (3) is equal to:

$$\sum_{i,k} \langle u_i | t_k \rangle \langle t_k | A | u_i \rangle = \sum_{i,k} \langle t_k | A | u_i \rangle \langle u_i | t_k \rangle \tag{4}$$

(since it is possible to change the order of two numbers in a product). We can then replace $\sum_i | u_i \rangle \langle u_i |$ in (4) by $\mathbb{1}$ (closure relation for the $| u_i \rangle$ states), and we obtain, finally:

$$\sum_i \langle u_i | A | u_i \rangle = \sum_k \langle t_k | A | t_k \rangle \tag{5}$$

We have therefore demonstrated the property of invariance for this case.

COMMENT:

If the operator A is an observable, Tr A can therefore be calculated in a basis of eigenvectors of A. The diagonal matrix elements are then the eigenvalues a_n of A (degree of degeneracy g_n) and the trace can be written:

$$\text{Tr}\, A = \sum_n g_n \, a_n \tag{6}$$

c. IMPORTANT PROPERTIES

$$\text{Tr}\, AB = \text{Tr}\, BA \tag{7a}$$
$$\text{Tr}\, ABC = \text{Tr}\, BCA = \text{Tr}\, CAB \tag{7b}$$

In general, the trace of the product of any number of operators is invariant when a cyclic permutation is performed on these operators.

Let us prove, for example, relation (7-a):

$$\begin{aligned}\text{Tr}\, AB &= \sum_i \langle u_i | AB | u_i \rangle = \sum_{i,j} \langle u_i | A | u_j \rangle \langle u_j | B | u_i \rangle \\ &= \sum_{i,j} \langle u_j | B | u_i \rangle \langle u_i | A | u_j \rangle = \sum_j \langle u_j | BA | u_j \rangle = \text{Tr}\, BA \end{aligned} \tag{8}$$

(twice using the closure relation on the $\{ | u_i \rangle \}$ basis). Relation (7-a) is thus proved; its generalization (7-b) presents no difficulty.

2. Commutator algebra

a. DEFINITION

The commutator $[A, B]$ of two operators is, by definition:

$$[A, B] = AB - BA \tag{9}$$

b. PROPERTIES

$$[A, B] = -[B, A] \tag{10}$$
$$[A, (B + C)] = [A, B] + [A, C] \tag{11}$$
$$[A, BC] = [A, B]C + B[A, C] \tag{12}$$
$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \tag{13}$$
$$[A, B]^\dagger = [B^\dagger, A^\dagger] \tag{14}$$

The derivation of these properties is straightforward : it suffices to compare both sides of each equation after having written them out explicitly.

3. Restriction of an operator to a subspace

Let P_q be the projector onto the q-dimensional subspace $\mathscr{E}_q$ spanned by the q orthonormal vectors $| \varphi_i \rangle$:

$$P_q = \sum_{i=1}^{q} | \varphi_i \rangle \langle \varphi_i | \tag{15}$$

By definition, the restriction $\hat{A}_q$ of the operator A to the subspace $\mathscr{E}_q$ is:

$$\hat{A}_q = P_q A P_q \tag{16}$$

If $| \psi \rangle$ is an arbitrary ket, it follows from this definition that:

$$\hat{A}_q | \psi \rangle = P_q A | \hat{\psi}_q \rangle \tag{17}$$

where:

$$| \hat{\psi}_q \rangle = P_q | \psi \rangle \tag{18}$$

is the orthogonal projection of $| \psi \rangle$ onto $\mathscr{E}_q$. Consequently, to make $\hat{A}_q$ act on an arbitrary ket $| \psi \rangle$, one begins by projecting this ket onto $\mathscr{E}_q$; then one lets the operator A act on this projection, retaining only the projection in $\mathscr{E}_q$ of the resulting ket. The operator $\hat{A}_q$, which transforms any ket of $\mathscr{E}_q$ into a ket belonging to this same subspace, is therefore an operator whose action has been restricted to $\mathscr{E}_q$.

What can be said about the matrix which represents $\hat{A}_q$? Let us choose a basis $\{ | u_k \rangle \}$ whose first q vectors belong to $\mathscr{E}_q$ (they are, for example, the $| \varphi_i \rangle$), the others belonging to the supplementary subspace. We have :

$$\langle u_i | \hat{A}_q | u_j \rangle = \langle u_i | P_q A P_q | u_j \rangle \tag{19}$$

that is:

$$\langle u_i | \hat{A}_q | u_j \rangle = \begin{cases} \langle u_i | A | u_j \rangle & \text{if } i, j \leq q \\ 0 & \text{if one of the two indices } i \text{ or } j \text{ is greater than } q \end{cases} \tag{20}$$

Therefore, the matrix which represents $\hat{A}_q$ is, as it were, "cut out" of the one which represents A. One retains only the matrix elements of A associated with basis vectors $| u_i \rangle$ and $| u_j \rangle$, both belonging to $\mathscr{E}_q$, the other matrix elements being replaced by zeros.

4. Functions of operators

a. DEFINITION; SIMPLE PROPERTIES

Consider an arbitrary linear operator A. It is not difficult to define the operator A^n: it is the operator which corresponds to n successive applications of the operator A. The definition of the operator A^{-1}, the inverse of A, is also well known : A^{-1} is the operator (if it exists) which satisfies the relations :

$$A^{-1}A = AA^{-1} = \mathbb{1} \tag{21}$$

How can we define, in a more general way, an arbitrary function of an operator? To do this, let us consider a function F of a variable z. Assume that, in a certain domain, F can be expanded in a power series in z:

$$F(z) = \sum_{n=0}^{\infty} f_n z^n \tag{22}$$

By definition, the corresponding function of the operator A is the operator $F(A)$ defined by a series which has the same coefficients f_n:

$$F(A) = \sum_{n=0}^{\infty} f_n A^n \tag{23}$$

For example, the operator e^A is defined by:

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!} = \mathbb{1} + A + A^2/2! + \ldots + A^n/n! + \ldots \tag{24}$$

We shall not consider the problems concerning the convergence of the series (23), which depends on the eigenvalues of A and on the radius of convergence of the series (22).

Note that if $F(z)$ is a real function, the coefficients f_n are real. If, moreover, A is Hermitian, we see from (23) that $F(A)$ is Hermitian.

Let $| \varphi_a \rangle$ be an eigenvector of A with eigenvalue a :

$$A | \varphi_a \rangle = a | \varphi_a \rangle \tag{25}$$

Applying the operator n times in succession, we obtain :

$$A^n | \varphi_a \rangle = a^n | \varphi_a \rangle \tag{26}$$

Now let us apply series (23) to $|\varphi_a\rangle$; we obtain:

$$F(A)|\varphi_a\rangle = \sum_{n=0}^{\infty} f_n a^n |\varphi_a\rangle = F(a)|\varphi_a\rangle \tag{27}$$

This leads to the following rule: *when $|\varphi_a\rangle$ is an eigenvector of A with the eigenvalue a, $|\varphi_a\rangle$ is also an eigenvector of $F(A)$, with the eigenvalue $F(a)$.*

This property leads to a second definition of a function of an operator. Let us consider a diagonalizable operator A (this is always the case if A is an observable), and let us choose a basis where the matrix associated with A is actually diagonal (its elements are then the eigenvalues a_i of A). $F(A)$ is, by definition, the operator which is represented, in this same basis, by the diagonal matrix whose elements are $F(a_i)$.

For example, if σ_z is the matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{28}$$

it follows directly that:

$$e^{\sigma_z} = \begin{pmatrix} e & 0 \\ 0 & 1/e \end{pmatrix} \tag{29}$$

COMMENT:

Care must be taken, when functions of operators are used, with respect to the order of the operators. For example, the operators $e^A e^B$, $e^B e^A$, and e^{A+B} are not, in general, equal when A and B are operators and not numbers. Consider:

$$e^A e^B = \sum_p \frac{A^p}{p!} \sum_q \frac{B^q}{q!} = \sum_{p,q} \frac{A^p}{p!} \frac{B^q}{q!} \tag{30}$$

$$e^B e^A = \sum_q \frac{B^q}{q!} \sum_p \frac{A^p}{p!} = \sum_{p,q} \frac{B^q A^p}{p!\,q!} \tag{31}$$

$$e^{A+B} = \sum_p \frac{(A+B)^p}{p!} \tag{32}$$

When A and B are arbitrary, the right-hand sides of (30), (31) and (32) have no reason to be equal (see exercise 7 of complement H_{II}). However, *when A and B commute*, we have:

$$[A, B] = 0 \Longrightarrow e^A e^B = e^B e^A = e^{A+B} \tag{33}$$

(a relation which is obvious, moreover, if the diagonal matrices which represent e^A and e^B are considered in a basis of eigenvectors common to A and B).

b. AN IMPORTANT EXAMPLE: THE POTENTIAL OPERATOR

In one-dimensional problems, we shall often have to consider "potential" operators $V(X)$ (so called because they correspond to the classical potential energy $V(x)$ of a particle placed in a force field), where $V(X)$ is a function of the position operator X.

It follows from the preceding section that $V(X)$ has as eigenvectors the eigenvectors $|x\rangle$ of X, and we have simply:

$$V(X)|x\rangle = V(x)|x\rangle \tag{34}$$

The matrix elements of $V(X)$ in the $\{|x\rangle\}$ representation are therefore:

$$\langle x|V(X)|x'\rangle = V(x)\delta(x-x') \tag{35}$$

Applying (34) and using the fact that $V(X)$ is Hermitian (the function $V(x)$ is real), we obtain:

$$\langle x|V(X)|\psi\rangle = V(x)\langle x|\psi\rangle = V(x)\psi(x) \tag{36}$$

This equation shows that in the $\{|x\rangle\}$ representation, the action of the operator $V(X)$ is simply multiplication by $V(x)$.

The generalization of (34), (35) and (36) to three-dimensional problems can be performed without difficulty; in this case, we obtain:

$$V(\mathbf{R})|\mathbf{r}\rangle = V(\mathbf{r})|\mathbf{r}\rangle \tag{37}$$

$$\langle \mathbf{r}|V(\mathbf{R})|\mathbf{r}'\rangle = V(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') \tag{38}$$

$$\langle \mathbf{r}|V(\mathbf{R})|\psi\rangle = V(\mathbf{r})\psi(\mathbf{r}) \tag{39}$$

c. COMMUTATORS INVOLVING FUNCTIONS OF OPERATORS

Definition (23) shows that A commutes with every function of A:

$$[A, F(A)] = 0 \tag{40}$$

Similarly, if A and B commute, so do $F(A)$ and B:

$$[B, A] = 0 \Longrightarrow [B, F(A)] = 0 \tag{41}$$

What will be the commutator of an operator with a function of another operator which does not commute with it? We shall restrict ourselves here to the case of the X and P operators, whose commutator is equal to:

$$[X, P] = i\hbar \tag{42}$$

Using relation (12), we can calculate:

$$[X, P^2] = [X, PP] = [X, P]P + P[X, P] = 2i\hbar\, P \tag{43}$$

More generally, let us show that:

$$[X, P^n] = i\hbar n P^{n-1} \tag{44}$$

If we assume that this equation is verified, we obtain:

$$\begin{aligned}[X, P^{n+1}] &= [X, PP^n] = [X, P]P^n + P[X, P^n] \\ &= i\hbar P^n + i\hbar n P P^{n-1} = i\hbar(n+1)P^n\end{aligned} \tag{45}$$

Relation (44) is therefore established by recurrence.

Now let us calculate the commutator $[X, F(P)]$:

$$[X, F(P)] = \sum_n [X, f_n P^n] = \sum_n i\hbar n f_n P^{n-1} \tag{46}$$

If $F'(z)$ denotes the derivative of the function $F(z)$, we recognize in (46) the definition of the operator $F'(P)$. Therefore:

$$\boxed{[X, F(P)] = i\hbar\, F'(P)} \tag{47}$$

An analogous argument would have enabled us to obtain the symmetric relation:

$$\boxed{[P, G(X)] = -\, i\hbar\, G'(X)} \tag{48}$$

COMMENTS:

(*i*) The preceding argument is based on the fact that $F(P)$ (or $G(X)$) depends only on P (or on X). It is more difficult to calculate a commutator such as $[X, \Phi(X, P)]$, where $\Phi(X, P)$ is an operator which depends on both X and P: the difficulties arise from the fact that X and P do not commute.

(*ii*) Equations (47) and (48) can be generalized to the case of two operators A and B which both commute with their commutator. An argument modeled on the preceding one shows that, if we have:

$$[A, C] = [B, C] = 0 \tag{49}$$

with $$C = [A, B] \tag{50}$$

then:

$$[A, F(B)] = [A, B]F'(B) \tag{51}$$

5. Differentiation of an operator

a. DEFINITION

Let $A(t)$ be an operator which depends on an arbitrary variable t. By definition, the derivative $\frac{dA}{dt}$ of $A(t)$ with respect to t is given by the limit (if it exists):

$$\frac{dA}{dt} = \lim_{\Delta t \to 0} \frac{A(t + \Delta t) - A(t)}{\Delta t} \tag{52}$$

The matrix elements of $A(t)$ in an arbitrary basis of t-independent vectors $| u_i \rangle$ are functions of t:

$$\langle u_i | A | u_j \rangle = A_{ij}(t) \tag{53}$$

Let us call $\left(\frac{dA}{dt}\right)_{ij} = \langle u_i \left| \frac{dA}{dt} \right| u_j \rangle$ the matrix elements of $\frac{dA}{dt}$. It is easy to verify the relation:

$$\left(\frac{dA}{dt}\right)_{ij} = \frac{d}{dt} A_{ij} \tag{54}$$

Thus we obtain a very simple rule: to obtain the matrix elements representing $\frac{dA}{dt}$ all we must do is take the matrix representing A and differentiate each of its elements (without changing their places).

b. DIFFERENTIATION RULES

They are analogous to the ones for ordinary functions:

$$\frac{d}{dt}(F + G) = \frac{dF}{dt} + \frac{dG}{dt} \tag{55}$$

$$\frac{d}{dt}(FG) = \frac{dF}{dt} G + F \frac{dG}{dt} \tag{56}$$

Nevertheless, care must be taken not to modify the order of the operators in formula (56).

Let us prove, for example, the second of these equations. The matrix elements of FG are:

$$\langle u_i | FG | u_j \rangle = \sum_k \langle u_i | F | u_k \rangle \langle u_k | G | u_j \rangle \tag{57}$$

We have seen that the matrix elements of $d(FG)/dt$ are the derivatives with respect to t of those of (FG). Thus we have, differentiating the right-hand side of (57):

$$\langle u_i | \frac{d}{dt}(FG) | u_j \rangle = \sum_k \Big[\langle u_i | \frac{dF}{dt} | u_k \rangle \langle u_k | G | u_j \rangle + \langle u_i | F | u_k \rangle \langle u_k | \frac{dG}{dt} | u_j \rangle \Big]$$
$$= \langle u_i | \frac{dF}{dt} G + F \frac{dG}{dt} | u_j \rangle \tag{58}$$

This equation is valid for any i and j. Formula (56) is thus established.

c. EXAMPLES

Let us calculate the derivative of the operator e^{At}. By definition, we have:

$$e^{At} = \sum_{n=0}^{\infty} \frac{(At)^n}{n!} \tag{59}$$

Differentiating the series term by term, we obtain:

$$\frac{d}{dt} e^{At} = \sum_{n=0}^{\infty} n \frac{t^{n-1}A^n}{n!}$$
$$= A \sum_{n=1}^{\infty} \frac{(At)^{n-1}}{(n-1)!}$$
$$= \left[\sum_{n=1}^{\infty} \frac{(At)^{n-1}}{(n-1)!} \right] A \qquad (60)$$

We recognize inside the brackets the series which defines e^{At} (taking as the summation index $p = n - 1$). The result is therefore:

$$\frac{d}{dt} e^{At} = A\,e^{At} = e^{At} A \qquad (61)$$

In this simple case involving only one operator, it is unnecessary to pay attention to the order of the factors : e^{At} and A commute.

This is not the case if one is interested in differentiating an operator such as $e^{At}e^{Bt}$. Applying (56) and (61), we obtain :

$$\frac{d}{dt} (e^{At} e^{Bt}) = A\,e^{At} e^{Bt} + e^{At} B\,e^{Bt} \qquad (62)$$

The right-hand side of this equation can be transformed into $e^{At}Ae^{Bt} + e^{At}Be^{Bt}$ or $e^{At}Ae^{Bt} + e^{At}e^{Bt}B$, for example. However, we can never obtain (unless, of course, A and B commute) an expression such as $(A + B)e^{At}e^{Bt}$. In this case, the order of the operators is therefore important.

COMMENT:

Even when the function involves only one operator, differentiation cannot always be performed according to the rules valid for ordinary functions. For example, when $A(t)$ has an arbitrary time-dependence, the derivative $\frac{d}{dt} e^{A(t)}$ *is generally not equal to* $\frac{dA}{dt} e^{A(t)}$. It can be seen by expanding $e^{A(t)}$ in a power series in $A(t)$ that $A(t)$ and $\frac{dA}{dt}$ must commute for this equality to hold.

d. AN APPLICATION: A USEFUL FORMULA

Consider two operators A and B which, by hypothesis, both commute with their commutator. In this case, we shall derive the relation:

$$e^A e^B = e^{A+B}\, e^{\frac{1}{2}[A,B]} \qquad (63)$$

(Glauber's formula).

Let us define the operator $F(t)$, a function of the real variable t, by:

$$F(t) = e^{At} e^{Bt} \qquad (64)$$

We have:

$$\frac{dF}{dt} = A\,e^{At} e^{Bt} + e^{At} B\,e^{Bt} = \left(A + e^{At} B\,e^{-At}\right) F(t) \qquad (65)$$

Since A and B commute with their commutator, formula (51) can be applied in order to calculate :

$$[e^{At}, B] = t[A, B]e^{At} \qquad (66)$$

Therefore:

$$e^{At}\,B = B\,e^{At} + t[A, B]e^{At} \qquad (67)$$

Multiply both sides of this equation on the right by e^{-At}. Substituting the relation so obtained into (65), we obtain:

$$\frac{dF}{dt} = \left(A + B + t[A, B]\right) F(t) \qquad (68)$$

The operators $A + B$ and $[A, B]$ commute by hypothesis. We can therefore integrate the differential equation (68) as if $A + B$ and $[A, B]$ were numbers. This yields:

$$F(t) = F(0)\, e^{(A+B)t + \frac{1}{2}[A,B]t^2} \qquad (69)$$

Setting $t = 0$, we see that $F(0) = \mathbb{1}$, and:

$$F(t) = e^{(A+B)t + \frac{1}{2}[A,B]t^2} \qquad (70)$$

Let us then set $t = 1$; we obtain equation (63), which is thus proven.

COMMENT :

When the operators A and B are arbitrary, equation (63) is not in general valid: it is necessary that both A and B commute with $[A, B]$. This condition may seem very restrictive. Actually, in quantum mechanics one often encounters operators whose commutator is a number: for example, X and P, or the operators a and $a^\dagger$ of the harmonic oscillator (*cf.* chap. V).

References :

See the subsections "General texts" and "Linear algebra – Hilbert spaces" of section 10 of the bibliography.

Complement C_{II}

UNITARY OPERATORS

1. General properties of unitary operators

a. DEFINITION; SIMPLE PROPERTIES

By definition, an operator U is unitary if its inverse U^{-1} is equal to its adjoint $U^\dagger$:

$$U^\dagger U = UU^\dagger = \mathbb{1} \tag{1}$$

Consider two arbitrary vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ of $\mathscr{E}$, and their transforms $|\tilde{\psi}_1\rangle$ and $|\tilde{\psi}_2\rangle$ under the action of U:

$$\begin{aligned} |\tilde{\psi}_1\rangle &= U|\psi_1\rangle \\ |\tilde{\psi}_2\rangle &= U|\psi_2\rangle \end{aligned} \tag{2}$$

Let us calculate the scalar product $\langle\tilde{\psi}_1|\tilde{\psi}_2\rangle$; we obtain:

$$\langle\tilde{\psi}_1|\tilde{\psi}_2\rangle = \langle\psi_1|U^\dagger U|\psi_2\rangle = \langle\psi_1|\psi_2\rangle \tag{3}$$

The unitary transformation associated with the operator U therefore conserves the scalar product (and, consequently, the norm) in $\mathscr{E}$. When $\mathscr{E}$ is finite-dimensional, moreover, this property is characteristic of a unitary operator.

COMMENTS:

(*i*) If A is a Hermitian operator, the operator $T = e^{iA}$ is unitary, since:

$$T^\dagger = e^{-iA^\dagger} = e^{-iA} \tag{4}$$

and therefore:

$$\begin{aligned} T^\dagger T &= e^{-iA}e^{iA} = \mathbb{1} \\ TT^\dagger &= e^{iA}e^{-iA} = \mathbb{1} \end{aligned} \tag{5}$$

(obviously, $-iA$ commutes with iA).

(*ii*) The product of two unitary operators is also unitary. If U and V are unitary, we have:

$$\begin{aligned} U^\dagger U &= UU^\dagger = \mathbb{1} \\ V^\dagger V &= VV^\dagger = \mathbb{1} \end{aligned} \tag{6}$$

Let us now calculate:

$$\begin{aligned} (UV)^\dagger(UV) &= V^\dagger U^\dagger UV = V^\dagger V = \mathbb{1} \\ (UV)(UV)^\dagger &= UVV^\dagger U^\dagger = UU^\dagger = \mathbb{1} \end{aligned} \tag{7}$$

These equations indeed show that the product operator UV is unitary. This property, moreover, was foreseeable: when two transformations conserve the scalar product, so does the successive application of these two transformations.

(*iii*) In the ordinary three-dimensional space of real vectors, we are familiar with operators which conserve the norm and the scalar product: rotations, symmetry operations with respect to a point, to a plane, etc. In this case where the space is real, these operators are said to be orthogonal. Unitary operators constitute the generalization of orthogonal operators to complex spaces (with an arbitrary number of dimensions).

b. UNITARY OPERATORS AND CHANGE OF BASES

α. Let $\{|v_i\rangle\}$ be an orthonormal basis of the state space $\mathscr{E}$, assumed to be discrete. Call $|\tilde{v}_i\rangle$ the transform of the vector $|v_i\rangle$ under the action of the operator U:

$$|\tilde{v}_i\rangle = U|v_i\rangle \tag{8}$$

Since the operator U is unitary, we have:

$$\langle\tilde{v}_i|\tilde{v}_j\rangle = \langle v_i|v_j\rangle = \delta_{ij} \tag{9}$$

The $|\tilde{v}_i\rangle$ vectors are therefore orthonormal. Let us show that they constitute a basis of $\mathscr{E}$. To do so, consider an arbitrary vector $|\psi\rangle$ of $\mathscr{E}$. Since the set $\{|v_i\rangle\}$ constitutes a basis, the vector $U^\dagger|\psi\rangle$ can be expanded on the $|v_i\rangle$:

$$U^\dagger|\psi\rangle = \sum_i c_i|v_i\rangle \tag{10}$$

Applying the operator U to this equation, we obtain:

$$UU^\dagger|\psi\rangle = \sum_i c_i U|v_i\rangle \tag{11}$$

and, therefore:

$$|\psi\rangle = \sum_i c_i|\tilde{v}_i\rangle \tag{12}$$

This equation expresses the fact that any vector $|\psi\rangle$ can be expanded on the vectors $|\tilde{v}_i\rangle$, which therefore constitute a basis. Thus we can state the following result: a necessary condition for an operator U to be unitary is that the vectors of an orthonormal basis of $\mathscr{E}$, transformed by U, constitute another orthonormal basis.

β. Conversely, let us show that this condition is sufficient. By hypothesis, we then have:

$$\begin{aligned} &|\,\tilde{v}_i\,\rangle = U\,|\,v_i\,\rangle \\ &\langle\,\tilde{v}_i\,|\,\tilde{v}_j\,\rangle = \delta_{ij} \\ &\sum_i |\,\tilde{v}_i\,\rangle\langle\,\tilde{v}_i\,| = \mathbb{1} \end{aligned} \tag{13}$$

and therefore:

$$\langle\,v_j\,|\,U^\dagger = \langle\,\tilde{v}_j\,| \tag{14}$$

Let us calculate:

$$\begin{aligned} U^\dagger U\,|\,v_i\,\rangle &= U^\dagger\,|\,\tilde{v}_i\,\rangle = \sum_j |\,v_j\,\rangle\langle\,v_j\,|\,U^\dagger\,|\,\tilde{v}_i\,\rangle \\ &= \sum_j |\,v_j\,\rangle\langle\,\tilde{v}_j\,|\,\tilde{v}_i\,\rangle = \sum_j |\,v_j\,\rangle\,\delta_{ij} \\ &= |\,v_i\,\rangle \end{aligned} \tag{15}$$

Relation (15), which is valid for all i, expresses the fact that the operator $U^\dagger U$ is the identity operator. Let us show, in the same way, that $UU^\dagger = \mathbb{1}$. To do this, consider the action of $U^\dagger$ on a vector $|\,v_i\,\rangle$:

$$\begin{aligned} U^\dagger\,|\,v_i\,\rangle &= \sum_j |\,v_j\,\rangle\langle\,v_j\,|\,U^\dagger\,|\,v_i\,\rangle \\ &= \sum_j |\,v_j\,\rangle\langle\,\tilde{v}_j\,|\,v_i\,\rangle \end{aligned} \tag{16}$$

We then have:

$$\begin{aligned} UU^\dagger\,|\,v_i\,\rangle &= \sum_j U\,|\,v_j\,\rangle\langle\,\tilde{v}_j\,|\,v_i\,\rangle \\ &= \sum_j |\,\tilde{v}_j\,\rangle\langle\,\tilde{v}_j\,|\,v_i\,\rangle \\ &= |\,v_i\,\rangle \end{aligned} \tag{17}$$

We deduce from this that $UU^\dagger = \mathbb{1}$: the operator U is therefore unitary.

c. UNITARY MATRICES

Let:

$$U_{ij} = \langle\,v_i\,|\,U\,|\,v_j\,\rangle \tag{18}$$

be the matrix elements of U. How can one see from the matrix representing U if this operator is unitary?

Relation (1) gives us:

$$\langle\,v_i\,|\,U^\dagger U\,|\,v_j\,\rangle = \sum_k \langle\,v_i\,|\,U^\dagger\,|\,v_k\,\rangle\langle\,v_k\,|\,U\,|\,v_j\,\rangle \tag{19}$$

that is:

$$\sum_k U^*_{ki}\,U_{kj} = \delta_{ij} \tag{20}$$

When a matrix is unitary, the sum of the products of the elements of one column and the complex conjugates of the elements of another column is

- zero if the two columns are different,
- equal to 1 if they are not.

Let us cite some examples in which this rule can be easily verified.

EXAMPLES:

(i) The matrix which represents a rotation through an angle θ about Oz, in ordinary three-dimensional space:

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{21}$$

(ii) The rotation matrix in the state space of a spin $\frac{1}{2}$ particle (*cf.* chap. IX):

$$R^{(1/2)}(\alpha, \beta, \gamma) = \begin{pmatrix} e^{-\frac{i}{2}(\alpha+\gamma)}\cos\dfrac{\beta}{2} & -\,e^{\frac{i}{2}(\gamma-\alpha)}\sin\dfrac{\beta}{2} \\ e^{\frac{i}{2}(\alpha-\gamma)}\sin\dfrac{\beta}{2} & e^{\frac{i}{2}(\alpha+\gamma)}\cos\dfrac{\beta}{2} \end{pmatrix} \tag{22}$$

d. EIGENVALUES AND EIGENVECTORS OF A UNITARY OPERATOR

Let $|\,\psi_u\,\rangle$ be a normalized eigenvector of the unitary operator U with eigenvalue u:

$$U\,|\,\psi_u\,\rangle = u\,|\,\psi_u\,\rangle \tag{23}$$

The square of the norm of the vector $U\,|\,\psi_u\,\rangle$ is:

$$\langle\,\psi_u\,|\,U^\dagger U\,|\,\psi_u\,\rangle = u^*u\,\langle\,\psi_u\,|\,\psi_u\,\rangle = u^*u \tag{24}$$

Since the unitary operator conserves the norm, we have, necessarily, $u^*u = 1$. The eigenvalues of a unitary operator must therefore be complex numbers of modulus 1:

$$u = e^{i\varphi_u} \quad \text{where } \varphi_u \text{ is real} \tag{25}$$

Consider two eigenvectors $|\,\psi_u\,\rangle$ and $|\,\psi_{u'}\,\rangle$ of U; we then have:

$$\begin{aligned} \langle\,\psi_u\,|\,\psi_{u'}\,\rangle &= \langle\,\psi_u\,|\,U^\dagger U\,|\,\psi_{u'}\,\rangle = u^*u'\,\langle\,\psi_u\,|\,\psi_{u'}\,\rangle \\ &= e^{i(\varphi_{u'}-\varphi_u)}\,\langle\,\psi_u\,|\,\psi_{u'}\,\rangle \end{aligned} \tag{26}$$

When the eigenvalues u and u' are different, we see from (26) that the scalar product $\langle\,\psi_u\,|\,\psi_{u'}\,\rangle$ is zero: two eigenvectors of a unitary operator corresponding to different eigenvalues are orthogonal.

2. Unitary transformations of operators

We saw in § 1-b that a unitary operator U permits the construction, starting with one orthonormal basis $\{ | v_i \rangle \}$ of $\mathscr{E}$, of another one, $\{ | \tilde{v}_i \rangle \}$. In this section, we are going to define a transformation which acts, not on the vectors, but on the operators.

By definition, the transform $\tilde{A}$ of the operator A will be the operator which, in the $\{ | \tilde{v}_i \rangle \}$ basis, has the same matrix elements as the operator A in the $\{ | v_i \rangle \}$ basis:

$$\langle \tilde{v}_i | \tilde{A} | \tilde{v}_j \rangle = \langle v_i | A | v_j \rangle \tag{27}$$

Substituting (8) into this equation, we obtain:

$$\langle v_i | U^\dagger \tilde{A} U | v_j \rangle = \langle v_i | A | v_j \rangle \tag{28}$$

Since i and j are arbitrary, we have:

$$U^\dagger \tilde{A} U = A \tag{29}$$

or, multiplying this equation on the left by U and on the right by $U^\dagger$:

$$\tilde{A} = U A U^\dagger \tag{30}$$

Equation (30) can be taken to be the definition of the transform $\tilde{A}$ of the operator A by the unitary transformation U. In quantum mechanics, such transformations are often used: a first example is given in complement F of this chapter (§ 2-a).

How can the eigenvectors of $\tilde{A}$ be obtained from those of A? Let us consider an eigenvector $| \varphi_a \rangle$ of A, with an eigenvalue a:

$$A | \varphi_a \rangle = a | \varphi_a \rangle \tag{31}$$

Let $| \tilde{\varphi}_a \rangle$ be the transform of $| \varphi_a \rangle$ by the operator U: $| \tilde{\varphi}_a \rangle = U | \varphi_a \rangle$. We then have:

$$\begin{aligned} \tilde{A} | \tilde{\varphi}_a \rangle &= (U A U^\dagger) U | \varphi_a \rangle = U A (U^\dagger U) | \varphi_a \rangle \\ &= U A | \varphi_a \rangle = a U | \varphi_a \rangle \\ &= a | \tilde{\varphi}_a \rangle \end{aligned} \tag{32}$$

$| \tilde{\varphi}_a \rangle$ is therefore an eigenvector of $\tilde{A}$, with eigenvalue a. This can be generalized to the following rule: the eigenvectors of the transform $\tilde{A}$ of A are the transforms $| \tilde{\varphi}_a \rangle$ of the eigenvectors $| \varphi_a \rangle$ of A; the eigenvalues are unchanged.

COMMENTS:

(*i*) The adjoint of the transform $\tilde{A}$ of A by U is the transform of $A^\dagger$ by U:

$$(\tilde{A})^\dagger = (U A U^\dagger)^\dagger = U A^\dagger U^\dagger = \widetilde{A^\dagger} \tag{33}$$

In particular, it follows from this equation that, if A is Hermitian, $\tilde{A}$ is also.

(*ii*) Analogously, we have:

$$(\tilde{A})^2 = U A U^\dagger U A U^\dagger = U A A U^\dagger = \widetilde{A^2}$$

and, in general:

$$(\tilde{A})^n = \widetilde{A^n} \tag{34}$$

Using definition (23) of complement B_{II}, we can easily show that:

$$\widetilde{F(A)} = F(\tilde{A}) \tag{35}$$

where $F(A)$ is a function of the operator A.

3. The infinitesimal unitary operator

Let $U(\varepsilon)$ be a unitary operator which depends on an infinitely small real quantity ε; by hypothesis, $U(\varepsilon) \longrightarrow \mathbb{1}$ when $\varepsilon \longrightarrow 0$. Expand $U(\varepsilon)$ in a power series in ε:

$$U(\varepsilon) = \mathbb{1} + \varepsilon G + \ldots \tag{36}$$

We then have:

$$U^\dagger(\varepsilon) = \mathbb{1} + \varepsilon G^\dagger + \ldots \tag{37}$$

and:

$$U(\varepsilon) U^\dagger(\varepsilon) = U^\dagger(\varepsilon) U(\varepsilon) = \mathbb{1} + \varepsilon(G + G^\dagger) + \ldots \tag{38}$$

Since $U(\varepsilon)$ is unitary, the first-order terms in ε on the right-hand side of (38) are zero; we therefore have:

$$G + G^\dagger = 0 \qquad G = -G^\dagger \tag{39}$$

This equation expresses the fact that the operator G is anti-Hermitian. It is convenient to set:

$$F = i G \tag{40}$$

so as to obtain the equation:

$$F - F^\dagger = 0 \tag{41}$$

which states that F is Hermitian. An infinitesimal unitary operator can therefore be written in the form:

$$U(\varepsilon) = \mathbb{1} - i \varepsilon F \tag{42}$$

where F is a Hermitian operator.

Substituting (42) into (30), we obtain:

$$\tilde{A} = (\mathbb{1} - i\varepsilon F) A (\mathbb{1} + i\varepsilon F^\dagger) = (\mathbb{1} - i\varepsilon F) A (\mathbb{1} + i\varepsilon F) \tag{43}$$

and, therefore:

$$\tilde{A} - A = - i \varepsilon [F, A] \tag{44}$$

The variation of the operator A under the transformation U is, to first order in ε, proportional to the commutator $[F, A]$.

Degeneracies may also arise which are not directly related to the symmetry of the problem. They are called *accidental degeneracies*. For example, in the case which we have discussed, it so happens that $E_{5,5} = E_{7,1}$ and $E_{7,4} = E_{8,1}$.

Complement H_{II}

EXERCISES

Dirac notation. Commutators. Eigenvectors and eigenvalues

1. $| \varphi_n \rangle$ are the eigenstates of a Hermitian operator H (H is, for example, the Hamiltonian of an arbitrary physical system). Assume that the states $| \varphi_n \rangle$ form a discrete orthonormal basis. The operator $U(m, n)$ is defined by:

$$U(m, n) = | \varphi_m \rangle \langle \varphi_n |$$

a. Calculate the adjoint $U^\dagger(m, n)$ of $U(m, n)$.

b. Calculate the commutator $[H, U(m, n)]$.

c. Prove the relation:

$$U(m, n)U^\dagger(p, q) = \delta_{nq}U(m, p)$$

d. Calculate Tr $\{ U(m, n) \}$, the trace of the operator $U(m, n)$.

e. Let A be an operator, with matrix elements $A_{mn} = \langle \varphi_m | A | \varphi_n \rangle$. Prove the relation:

$$A = \sum_{m,n} A_{mn}\, U(m, n)$$

f. Show that $A_{pq} = \text{Tr} \{ AU^\dagger(p, q) \}$.

2. In a two-dimensional vector space, consider the operator whose matrix, in an orthonormal basis $\{ | 1 \rangle, | 2 \rangle \}$, is written:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

a. Is σ_y Hermitian? Calculate its eigenvalues and eigenvectors (giving their normalized expansion in terms of the $\{ | 1 \rangle, | 2 \rangle \}$ basis).

b. Calculate the matrices which represent the projectors onto these eigenvectors. Then verify that they satisfy the orthogonality and closure relations.

c. Same questions for the matrices:

$$M = \begin{pmatrix} 2 & i\sqrt{2} \\ -i\sqrt{2} & 3 \end{pmatrix}$$

and, in a three-dimensional space

$$L_y = \frac{\hbar}{2i}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}$$

3. The state space of a certain physical system is three-dimensional. Let $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ be an orthonormal basis of this space. The kets $|\psi_0\rangle$ and $|\psi_1\rangle$ are defined by:

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}|u_1\rangle + \frac{i}{2}|u_2\rangle + \frac{1}{2}|u_3\rangle$$

$$|\psi_1\rangle = \frac{1}{\sqrt{3}}|u_1\rangle + \frac{i}{\sqrt{3}}|u_3\rangle$$

a. Are these kets normalized?

b. Calculate the matrices ρ_0 and ρ_1 representing, in the $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis, the projection operators onto the state $|\psi_0\rangle$ and onto the state $|\psi_1\rangle$. Verify that these matrices are Hermitian.

4. Let K be the operator defined by $K = |\varphi\rangle\langle\psi|$, where $|\varphi\rangle$ and $|\psi\rangle$ are two vectors of the state space.

a. Under what condition is K Hermitian?

b. Calculate K^2. Under what condition is K a projector?

c. Show that K can always be written in the form $K = \lambda P_1 P_2$ where λ is a constant to be calculated and P_1 and P_2 are projectors.

5. Let P_1 be the orthogonal projector onto the subspace $\mathscr{E}_1$, P_2 the orthogonal projector onto the subspace $\mathscr{E}_2$. Show that, for the product P_1P_2 to be an orthogonal projector as well, it is necessary and sufficient that P_1 and P_2 commute. In this case, what is the subspace onto which P_1P_2 projects?

6. The σ_x matrix is defined by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Prove the relation:

$$e^{i\alpha\sigma_x} = I\cos\alpha + i\sigma_x \sin\alpha$$

where I is the 2×2 unit matrix.

7. Establish, for the σ_y matrix given in exercise 2, a relation analogous to the one proved for σ_x in the preceding exercise. Generalize for all matrices of the form:

$$\sigma_u = \lambda\sigma_x + \mu\sigma_y$$

with:

$$\lambda^2 + \mu^2 = 1$$

Calculate the matrices representing $e^{2i\sigma_x}$, $(e^{i\sigma_x})^2$ and $e^{i(\sigma_x+\sigma_y)}$. Is $e^{2i\sigma_x}$ equa to $(e^{i\sigma_x})^2$? $e^{i(\sigma_x+\sigma_y)}$ to $e^{i\sigma_x}e^{i\sigma_y}$?

8. Consider the Hamiltonian H of a particle in a one-dimensional problen defined by:

$$H = \frac{1}{2m}P^2 + V(X)$$

where X and P are the operators defined in § E of chapter II and which satisfy th relation: $[X, P] = i\hbar$. The eigenvectors of H are denoted by $|\varphi_n\rangle$: $H|\varphi_n\rangle = E_n|\varphi_n\rangle$ where n is a discrete index.

a. Show that:

$$\langle\varphi_n|P|\varphi_{n'}\rangle = \alpha\langle\varphi_n|X|\varphi_{n'}\rangle$$

where α is a coefficient which depends on the difference between E_n and $E_{n'}$. Calculate α (hint: consider the commutator $[X, H]$).

b. From this, deduce, using the closure relation, the equation:

$$\sum_{n'}(E_n - E_{n'})^2|\langle\varphi_n|X|\varphi_{n'}\rangle|^2 = \frac{\hbar^2}{m^2}\langle\varphi_n|P^2|\varphi_n\rangle$$

notice the order

9. Let H be the Hamiltonian operator of a physical system. Denote by $|\varphi_n\rangle$ the eigenvectors of H, with eigenvalues E_n:

$$H|\varphi_n\rangle = E_n|\varphi_n\rangle$$

a. For an arbitrary operator A, prove the relation:

$$\langle\varphi_n|[A, H]|\varphi_n\rangle = 0.$$

b. Consider a one-dimensional problem, where the physical system is a particle of mass m and of potential energy $V(X)$. In this case, H is written:

$$H = \frac{1}{2m}P^2 + V(X)$$

α. In terms of P, X and $V(X)$, find the commutators: $[H, P]$, $[H, X]$ and $[H, XP]$.

β. Show that the matrix element $\langle\varphi_n|P|\varphi_n\rangle$ (which we shall interpret in chapter III as the mean value of the momentum in the state $|\varphi_n\rangle$) is zero.

γ. Establish a relation between $E_k = \langle\varphi_n|\frac{P^2}{2m}|\varphi_n\rangle$ (the mean value of the kinetic energy in the state $|\varphi_n\rangle$) and $\langle\varphi_n|X\frac{dV}{dX}|\varphi_n\rangle$. Since the mean value of the potential energy in the state $|\varphi_n\rangle$ is $\langle\varphi_n|V(x)|\varphi_n\rangle$, how is it related to the mean value of the kinetic energy when:

$$V(X) = V_0 X^\lambda$$

$(\lambda = 2, 4, 6 \ldots; V_0 > 0)$?

10 Using the relation $\langle x | p \rangle = (2\pi\hbar)^{-1/2} e^{ipx/\hbar}$, find the expressions $\langle x | XP | \psi \rangle$ and $\langle x | PX | \psi \rangle$ in terms of $\psi(x)$. Can these results be found directly by using the fact that in the $\{ | x \rangle \}$ representation, P acts like $\frac{\hbar}{i}\frac{d}{dx}$?

Sets of commuting observables and C.S.C.O.'S

11. Consider a physical system whose three-dimensional state space is spanned by the orthonormal basis formed by the three kets $| u_1 \rangle, | u_2 \rangle, | u_3 \rangle$. In the basis of these three vectors, taken in this order, the two operators H and B are defined by:

$$H = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad B = b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

where ω_0 and b are real constants.

a. Are H and B Hermitian?

b. Show that H and B commute. Give a basis of eigenvectors common to H and B.

c. Of the sets of operators: $\{ H \}, \{ B \}, \{ H, B \}, \{ H^2, B \}$, which form a C.S.C.O.?

12. In the same state space as that of the preceding exercise, consider two operators L_z and S defined by:

$$L_z | u_1 \rangle = | u_1 \rangle \qquad L_z | u_2 \rangle = 0 \qquad L_z | u_3 \rangle = -| u_3 \rangle$$
$$S | u_1 \rangle = | u_3 \rangle \qquad S | u_2 \rangle = | u_2 \rangle \qquad S | u_3 \rangle = | u_1 \rangle$$

a. Write the matrices which represent, in the $\{ | u_1 \rangle, | u_2 \rangle, | u_3 \rangle \}$ basis, the operators L_z, L_z^2, S, S^2. Are these operators observables?

b. Give the form of the most general matrix which represents an operator which commutes with L_z. Same question for L_z^2, then for S^2.

c. Do L_z^2 and S form a C.S.C.O.? Give a basis of common eigenvectors.

Solution of exercise 11

a. H and B are Hermitian because the matrices which correspond to the are symmetric and real.

b. $| u_1 \rangle$ is an eigenvector common to H and B. We therefore have, obviousl $HB | u_1 \rangle = BH | u_1 \rangle$. We see, then, that for H and B to commute, it is sufficie that the restrictions of these operators to the subspace $\mathscr{E}_2$, spanned by $| u_2$ and $| u_3 \rangle$, commute. Now, in this subspace, the matrix representing H is equ to $-\hbar\omega_0 I$ (where I is the 2×2 unit matrix), which commutes with all 2×2 matrice H and B therefore commute (this result could, of course, be obtained by calcı lating directly the matrices HB and BH). The restriction of B to $\mathscr{E}_2$ is written

$$P_{\mathscr{E}_2} B P_{\mathscr{E}_2} = b \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The normalized eigenvectors of this 2×2 matrix are easy to obtain; they are:

$$| p_2 \rangle = \frac{1}{\sqrt{2}} [| u_2 \rangle + | u_3 \rangle] \qquad \text{(eigenvalue } + b)$$

$$| p_3 \rangle = \frac{1}{\sqrt{2}} [| u_2 \rangle - | u_3 \rangle] \qquad \text{(eigenvalue } - b)$$

These vectors are automatically eigenvectors of H since $\mathscr{E}_2$ is the eigensubspa of H corresponding to the eigenvalue $-\hbar\omega_0$. To summarize, the eigenvecto common to H and B are given by:

	eigenvalue of H	eigenvalue of B
$\vert p_1 \rangle = \vert u_1 \rangle$	$\hbar\omega_0$	b
$\vert p_2 \rangle = \frac{1}{\sqrt{2}} [\vert u_2 \rangle + \vert u_3 \rangle]$	$-\hbar\omega_0$	b
$\vert p_3 \rangle = \frac{1}{\sqrt{2}} [\vert u_2 \rangle - \vert u_3 \rangle]$	$-\hbar\omega_0$	$-b$

These vectors are the only (to within, of course, a phase factor) normalized eigen vectors common to H and B.

c. It can be seen from the table that H has a two-fold degenerat eigenvalue; it is therefore not a C.S.C.O. Similarly, B also has a two-fold degenerat eigenvalue and is therefore not a C.S.C.O.: an eigenvector of B with th eigenvalue b can be $| p_1 \rangle$, or $| p_2 \rangle$, or $\frac{1}{\sqrt{3}} | u_1 \rangle + \frac{1}{\sqrt{3}} | u_2 \rangle + \frac{1}{\sqrt{3}} | u_3 \rangle$, fo example. On the other hand, the set of the two operators H and B does constitut a C.S.C.O. We see from the above table that no two vectors $| p_j \rangle$ have the sam eigenvalues for both H and B. This is why, as has already been pointed out, th system of normalized eigenvectors common to H and B is unique (to within phas factors). Note that within the eigensubspace $\mathscr{E}_2$ of H associated with the eigen value $-\hbar\omega_0$, the eigenvalues of B are distinct (b and $-b$). Similarly, in th eigensubspace of B spanned by $| p_1 \rangle$ and $| p_2 \rangle$, the eigenvalues of H are distinct ($\hbar\omega_0$ and $-\hbar\omega_0$).

H^2 has for eigenvectors, with the eigenvalue $\hbar^2\omega_0^2$, $| p_1 \rangle$, $| p_2 \rangle$ and $| p_3 \rangle$. It is easy to see that H^2 and B do not constitute a C.S.C.O., since two linearly independent eigenvectors $| p_1 \rangle$ and $| p_2 \rangle$ correspond to the pair of eigenvalues $\{ \hbar^2\omega_0^2, b \}$.

Solution of exercise 12

a. Let us use the rule for constructing the matrix of an operator : "in the nth column of the matrix, write the components of the operator transform of the nth basis vector". We obtain easily :

$$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad S = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$L_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad S^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

These matrices are symmetric and real, and therefore Hermitian. Since the space is finite-dimensional, they can be diagonalized and therefore represent observables.

b. Let M be an operator which commutes with L_z. M cannot (*cf.* chap. II, §D-3-a) have any matrix elements between $| u_1 \rangle$ and $| u_2 \rangle$, or between $| u_2 \rangle$ and $| u_3 \rangle$, or between $| u_1 \rangle$ and $| u_3 \rangle$ (eigenvectors of L_z with different eigenvalues). The matrix which represents M is therefore necessarily diagonal, that is, of the form:

$$[M, L_z] = 0 \quad \Longleftrightarrow \quad M = \begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}$$

Let N be an operator which commutes with L_z^2. The matrix representing N can have elements between $| u_1 \rangle$ and $| u_3 \rangle$ (eigenvectors of L_z^2 with the same eigenvalue), but none between $| u_2 \rangle$ and $| u_1 \rangle$ or $| u_3 \rangle$. N is therefore written:

$$[N, L_z^2] = 0 \quad \Longleftrightarrow \quad N = \begin{pmatrix} n_{11} & 0 & n_{13} \\ 0 & n_{22} & 0 \\ n_{31} & 0 & n_{33} \end{pmatrix}$$

It is therefore less restrictive to impose the condition that an operator commute with L_z^2 than with L_z : N is not necessarily a diagonal matrix. It can only be said that N does not mix the vectors of the subspace $\mathscr{F}_2$ spanned by $| u_1 \rangle$ and $| u_3 \rangle$ with those of the one-dimensional subspace spanned by $| u_2 \rangle$. This property,

moreover, appears very clearly if the matrix N' which represents the operator is written in the $\{ | u_1 \rangle, | u_3 \rangle, | u_2 \rangle \}$ basis (changing the order of the basis vectors

$$N' = \begin{pmatrix} n_{11} & n_{13} & 0 \\ n_{31} & n_{33} & 0 \\ 0 & 0 & n_{22} \end{pmatrix}$$

Finally, since S^2 is the identity operator, any 3×3 matrix commutes with S^2, a
its most general form is:

$$[P, S^2] = 0 \quad \Longleftrightarrow \quad P = \begin{pmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{pmatrix}$$

c. $| u_2 \rangle$ is an eigenvector common to L_z^2 and S. In the subspace $\mathscr{F}_2$ spann
by $| u_1 \rangle$ and $| u_3 \rangle$, L_z^2 and S are written:

$$P_{\mathscr{F}_2} L_z^2 P_{\mathscr{F}_2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$P_{\mathscr{F}_2} S P_{\mathscr{F}_2} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The eigenvectors of the latter matrix are:

$$| q_2 \rangle = \frac{1}{\sqrt{2}} [| u_1 \rangle + | u_3 \rangle]$$

$$| q_3 \rangle = \frac{1}{\sqrt{2}} [| u_1 \rangle - | u_3 \rangle]$$

and the basis of eigenvectors common to L_z^2 and S is:

vector	eigenvalue of L_z^2	eigenvalue of S
$\lvert q_1 \rangle = \lvert u_2 \rangle$	0	1
$\lvert q_2 \rangle = \frac{1}{\sqrt{2}} [\lvert u_1 \rangle + \lvert u_3 \rangle]$	1	1
$\lvert q_3 \rangle = \frac{1}{\sqrt{2}} [\lvert u_1 \rangle - \lvert u_3 \rangle]$	1	-1

No two lines are alike in the table of eigenvalues of L_z^2 and S : these two operato
therefore form a C.S.C.O. (this is not, however, the case for either one of the
taken alone).