Normal Form of Antiunitary Operators

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Antiunitary operators are characterized in a manner similar to the characterization of unitary operators by their characteristic vectors and characteristic values. It is shown that a complete orthonormal set of vectors can be defined, some of which are invariant under the antiunitary operator. The rest of the vectors, which are always even in number, form pairs in such a way that the antiunitary operator transforms each member of a pair into a multiple of the other member of the same pair [Eq. (11)]. The extent to which the vectors of the orthonormal set are determined by the antiunitary operator is ascertained and the number of free parameters in the various cases of degeneracy found.

1.

ANTIUNITARY operators[1] play a significant role in the theory of the invariance of quantum mechanical equations. The symmetry operators which involve the operation of time-inversion are antiunitary. The antiunitary operators are antilinear, i.e., if φ and ψ are two vectors of the complex Hilbert space in which the antiunitary operator A is defined and if a and b are two complex numbers,

$$A(a\varphi+b\psi)=a^*A\varphi+b^*A\psi. \tag{1}$$

The asterisk denotes the conjugate complex. Furthermore, A changes the scalar product into its conjugate complex

$$(A\varphi,A\psi)=(\varphi,\psi)^*=(\psi,\varphi). \tag{2}$$

Actually, (1) follows from (2) so that the latter equation can serve as the definition of the antiunitary nature of A. However, unless the Hilbert space has only a finite number of dimensions, it is also necessary to specify that A has an inverse. This is also antiunitary.

If A is antiunitary, A^2 defined by

$$A^2\psi=A(A\psi) \tag{3}$$

is unitary. This follows directly from the defining Eqs. (1) and (2), and it is also clear that A^2 has an inverse if A does.

If Av_k is given for all the members of a complete orthonormal set of vectors $v_1,v_2,\cdots$, its antilinear property defines it for all vectors $v=\Sigma a_k v_k$:

$$Av=A(\sum a_k v_k)=\sum a_k^* A v_k. \tag{4}$$

Hence, the normal form of A will be obtained by specifying a complete set of orthonormal vectors v_k for which Av_k has a particularly simple form. These vectors are the analogs of the characteristic vectors for unitary operators and will be, indeed, characteristic vectors of A^2. However, this property does not define them completely.

If $v_1,v_2,\cdots$ form a complete orthonormal set, $Av_1,Av_2,\cdots$ also form such a set. The orthonormal nature of the latter set follows directly from (2), the completeness from the existence of the inverse of A. If w were orthogonal to all Av_k, then $A^{-1}w$ would be orthogonal to all v_k.

We mention further for the sake of completeness, that if K is the operation of complex conjugation so that, in a particular coordinate system,

$$K\psi=\psi^*;\quad K^2=1, \tag{5}$$

AK is unitary and it follows that every antiunitary operator can be written in the form

$$A=UK, \tag{6}$$

where U is unitary. It follows from (6) that

$$A^2=UKUK=UU^*K^2=UU^*, \tag{7}$$

where U^* is the conjugate complex of U in the coordinate system in which (5) is valid. Since UU^* is equivalent to its conjugate complex

$$UU^*=UU^*UU^{-1}=U(UU^*)^*U^{-1}, \tag{8}$$

its characteristic values are either real or pairwise conjugate complex. It follows that the square of an antiunitary operator is equivalent to a rotation. The last four equations will not be used explicitly.

2.

It will be assumed that the spectrum of $A^2=\Lambda$ is discrete. The complications which arise if Λ has a continuous spectrum are not serious, but their elimination is cumbersome. Let us consider then a characteristic vector of Λ:

$$\Lambda v=A^2v=\omega v. \tag{9}$$

Since Λ is unitary, $|\omega|=1$. It then follows that Av is also a characteristic vector of Λ,

$$\Lambda Av=A^2Av=AA^2v=A\omega v=\omega^*Av, \tag{10}$$

[1] Some of the results of the present article can be obtained on the basis of theorems derived by E. Cartan in his *Lecons sur la Géométrie Projective Complexe* (Gauthier-Villars, Paris, 1931). I am much indebted to Professor S. Bochner for drawing my attention to the very profound investigations contained in this treatise, which deals with general linear and antilinear transformations. However, the direct derivations, given in the text of the present paper, are hardly longer than the reinterpretation and amplification of Cartan's results (see particularly pp. 124–137) would have been.

and belongs to the characteristic value ω^*. Unless $\omega=1$ or $\omega=-1$, $\omega\neq\omega^*$ and Av is orthogonal to v. Hence, if we choose an arbitrary orthonormal base, $v_{\omega 1}, v_{\omega 2}, \cdots$ among the characteristic vectors of ω, we can define, if ω is complex,

$$v_{\omega^*,k}=\omega^{\frac{1}{2}}Av_{\omega,k} \quad \text{or} \quad Av_{\omega,k}=(\omega^{\frac{1}{2}})^*v_{\omega^*k} \qquad (11)$$

and the $v_{\omega^*,k}$ will form a full base of orthonormal characteristic vectors to ω^*. The sign of the square root in (11) is best fixed in such a way that the imaginary part of $\omega^{\frac{1}{2}}$ shall have the same sign as the imaginary part of ω. Then $(\omega^*)^{\frac{1}{2}}=(\omega^{\frac{1}{2}})^*$. The purpose of the $\omega^{\frac{1}{2}}$ factor will become evident at once.

Application of A to both sides of (11) gives

$$Av_{\omega^*,k}=(\omega^{\frac{1}{2}})^*A^2v_{\omega,k}=(\omega^{\frac{1}{2}})^*\omega v_{\omega,k}=\omega^{\frac{1}{2}}v_{\omega,k}, \qquad (12)$$

so that the choice of the characteristic vectors to ω^* made in (11) renders this equation valid also if ω is replaced by ω^*. The $v_{\omega,k}$ may be called characteristic vectors of A also.[2] However, in contrast to the unitary case, the characteristic vectors of A to ω also define the characteristic vectors of A to ω^* if we want (11) to hold. If one recalls that Λ is equivalent to a rotation it is not surprising that a certain amount of simplification results if a relation exists between the characteristic vectors of ω and of ω^*. In the case of a rotation one would set $v_{\omega^*,k}=v_{\omega,k}^*$.

Let us consider now a characteristic vector v to the characteristic value 1:

$$\Lambda v=A^2v=v. \qquad (13)$$

It then follows from (10) that Av is also a characteristic vector to the characteristic value 1 and so is, unless it vanishes, $v_{11}=c(v+Av)$; c is a real normalization constant. It follows from (13) that

$$Av_{11}=Ac(v+Av)=c(Av+v)=v_{11}, \qquad (14)$$

so that v_{11} is invariant under A. If $v=-Av$ we choose $v_{11}=iv$ and have again

$$Av_{11}=Aiv=-iAv=iv=v_{11}. \qquad (15)$$

Next we consider another characteristic vector $v'=\Lambda v'$ which is orthogonal to v_{11}:

$$(v_{11},v')=0. \qquad (16)$$

Because of (2) and (14),

$$(v_{11},Av')=(A^2v',Av_{11})=(\Lambda v',v_{11})=(v',v_{11})=0, \qquad (17)$$

Av' will also be orthogonal to v_{11}. We can write therefore $v_{12}=c(v'+Av')$ or, if this vanishes, $v_{12}=iv'$, and this will still be orthogonal to v_{11} and also invariant under A. Proceeding in the same way, a full orthonormal base $v_{11}, v_{12}, \cdots$ of characteristic vectors of Λ to the characteristic value 1 can be found which are invariant under A,

$$Av_{1k}=v_{1k}. \qquad (18)$$

The vectors which satisfy (18) can be called the invariant vectors of A. The procedure just used to ensure (18) is similar to the separation of real and imaginary parts of a number.

Let us finally consider a characteristic vector of Λ to -1:

$$\Lambda v_{-11}=A^2v_{-11}=-v_{-11}. \qquad (19)$$

In this case again, because of (10), Av_{-11} is also a characteristic value to -1. Furthermore, Av_{-11} is orthogonal to v_{-11} because of (2) and (19):

$$(v_{-11},Av_{-11})=(A^2v_{-11},Av_{-11})=-(v_{-11},Av_{-11}). \qquad (20)$$

Hence we can write

$$v_{-1^*1}=iAv_{-11} \quad v_{-11}=i^*Av_{-1^*1}=-iAv_{-1^*1}. \qquad (21)$$

If Λ has further linearly independent characteristic vectors to -1, a normalized v_{-12} can be found which is orthogonal to both v_{-11} and v_{-1^*1}. Furthermore, the same will be true of $v_{-1^*2}=iAv_{-12}$. Thus, for instance,

$$(v_{-1^*2},v_{-11})=(iAv_{-12},v_{-11})=-i(Av_{-11},A^2v_{-12})$$
$$=-i(-iv_{-1^*1},-v_{-12})=0. \qquad (22)$$

Hence, proceeding in the same way, one can find a full orthonormal base of characteristic vectors of Λ to -1,

$$\Lambda v_{-1k}=-v_{-1k} \quad \Lambda v_{-1^*k}=-v_{-1^*k}, \qquad (23)$$

for which

$$v_{-1^*k}=iAv_{-1k} \quad v_{-1k}=-iAv_{-1^*k}=i^*A_{-1^*k} \qquad (24)$$

holds. These equations are formally identical with the Eqs. (11) for complex characteristic values if one considers -1 to be two conjugate complex characteristic values -1 and -1^* of Λ, which happen to coincide. The v_{-1k} belong to the characteristic value -1, the v_{-1^*k} to the characteristic value -1^*. Equation (24) becomes a special case of (11) if one sets $(-1)^{\frac{1}{2}}=i$; $(-1^*)^{\frac{1}{2}}=i^*=-i$.

3.

On summarizing the preceding results, we can characterize an antiunitary operator by two sets of vectors, which jointly form a complete orthonormal set, together with the characteristic values $\omega_1, \omega_1^*, \omega_2, \omega_2^*, \cdots$ belonging to the second set. These characteristic values are pairwise conjugate complex, of modulus 1, but are not equal to 1. The first set of vectors are invariant under the antiunitary operator, i.e., (18) applies to them; (11) is valid for the members of the second set. The ω may also be equal to -1, but this characteristic value always occurs in pairs and one member of the pair is denoted by -1, the other by -1^*.

It will be shown now that any two sets of vectors v_{1k} and $v_{\omega k}$ which jointly form a complete orthonormal

[2] The two vectors $v_{\omega k}$ and $v_{\omega^* k}$ form a plane in our Hilbert space. The line which corresponds to this plane in Cartan's projective space is the invariant line of the passage cited in footnote reference 1.

set, together with the corresponding ω, give an antiunitary operator by means of (4), (11), and (18). In other words, the sets v_{1k} and $v_{\omega k}$ are not subject to any further conditions except that there are just as many vectors bearing the index ω as there are with the index ω^*. The number of vectors in the first set is arbitrary and so are the values of ω except that $\omega\neq 1$, $|\omega|=1$ and they occur in conjugate complex pairs.

In order to prove the preceding assertion we consider two vectors φ and ψ and expand them in terms of the orthonormal set

$$\varphi=\sum_k a_k v_{1k}+\sum_{\omega k} b_{\omega k}v_{\omega k}$$
$$\psi=\sum_k c_k v_{1k}+\sum_{\omega k} d_{\omega k}v_{\omega k}. \tag{25}$$

$A\varphi$ and $A\psi$ are then given by

$$A\varphi=\sum_k a_k^* v_{1k}+\sum_{\omega k} b_{\omega k}^*(\omega^{\frac{1}{2}})^* v_{\omega^* k}$$
$$A\psi=\sum_k c_k^* v_{1k}+\sum_{\omega k} d_{\omega k}^*(\omega^{\frac{1}{2}})^* v_{\omega^* k}. \tag{26}$$

Both conditions (1) and (2) of the antiunitary nature of A can be verified to be consequences of (26) and the orthonormality of the v_{1k}, $v_{\omega k}$, provided that

$$(\omega^*)^{\frac{1}{2}}=(\omega^{\frac{1}{2}})^* \quad |\omega|=1. \tag{27}$$

For $\omega=-1$, this last condition is spelled out explicitly in (23). As was mentioned before, (27) can most simply be assured for complex ω by using that sign for $\omega^{\frac{1}{2}}$ for which the signs of the imaginary parts of ω and of $\omega^{\frac{1}{2}}$ are the same.

4.

Evidently, the two sets v_{1k}, $v_{\omega k}$ and the corresponding ω completely determine A. Conversely, A determines the number of vectors contained in the set v_{1k}—this is the multiplicity of the characteristic value 1 of A^2—and the value of the ω and their multiplicities. However, the vectors v are not completely determined by A and the present section will be devoted to the determination of the freedom that remains in the choice of these vectors.

Let us denote two other orthonormal sets which characterize the same antilinear operator by w_{1k} and $w_{\omega k}$. Since the w_{1k} form a base for the characteristic functions to the characteristic value 1 of $\Lambda=A^2$, they are connected with the v_{1k} by a nonsingular transformation

$$w_{1k}=\sum r_{kl}v_{1l}. \tag{28}$$

In fact, it follows from the orthonormality of the v_{1k} and of the w_{1k} that r is unitary. This is, however, not the only condition on r: If the vectors w_{1k} are to be invariant under A, i.e., if they satisfy (18),

$$Aw_{1k}=\sum r_{kl}^* Av_{1l}=\sum r_{kl}^* v_{1l}=w_{1k}, \tag{29}$$

the r_{kl} must be real. Hence, two different invariant sets of vectors of the same antiunitary operator are related to each other by a rotation

$$r=r^* \quad rr'=rr^\dagger=1. \tag{30}$$

The prime denotes the transpose, the dagger the Hermitian adjoint.

For complex ω, the sets $w_{\omega k}$ and $v_{\omega k}$ span the same linear manifold. Hence, we have

$$w_{\omega k}=\sum u_{kl}^{(\omega)}v_{\omega l}, \tag{31}$$

and it again follows from the orthonormality of the w_ω and v_ω that $u^{(\omega)}$ is unitary. By calculating $Aw_{\omega k}$ again, we find

$$Aw_{\omega k}=\sum u_{kl}^{(\omega)*}Av_{\omega l}=\sum u_{kl}^{(\omega)*}(\omega^*)^{\frac{1}{2}}v_{\omega^* l}, \tag{32}$$

so that if we want $Aw_{\omega k}=(\omega^*)^{\frac{1}{2}}w_{\omega^* k}$ to remain valid, we must have

$$u^{(\omega^*)}=u^{(\omega)*}, \tag{33}$$

i.e., the unitary transformations which belong to conjugate complex characteristic value are conjugate complex.

The preceding argument does not apply if $\omega=-1$. It is indeed clear that in this case the w_{-1k} may be linear combinations of the v_{-1k} and of the v_{-1^*k} because all these belong to the characteristic value -1 of Λ. Hence we set

$$w_{-1k}=\sum s_{kl}v_{-1l}+\sum t_{kl}v_{-1^*l}. \tag{34}$$

The condition (24) that $w_{-1^*k}=iAw_{-1k}$ now reads

$$\begin{aligned} w_{-1^*k}&=iA\left(\sum s_{kl}v_{-1l}+\sum t_{kl}v_{-1^*l}\right)\\ &=\sum s_{kl}^*iAv_{-1l}+\sum t_{kl}^*iAv_{-1^*l}\\ &=\sum -t_{kl}^*v_{-1l}+\sum s_{kl}^*v_{-1^*l}. \end{aligned} \tag{35}$$

Hence, the sets of vectors w_{-1} and w_{-1^*} are obtained from the sets v_{-1}, v_{-1^*} by the transformation

$$S=\left\|\begin{matrix} s & t \\ -t^* & s^* \end{matrix}\right\|. \tag{36}$$

This will guarantee that (24) is valid for the w_{-1}, w_{-1^*} if it is valid for the v_{-1}, v_{-1^*} because the second set of Eqs. (24) can be obtained from the first set by applying A to these. However, in order to make the w_{-1}, w_{-1^*} an orthonormal set, the S of (36) must be unitary. The conditions for this are obtained by setting $SS^\dagger=1$ or, in terms of the submatrices s and t,

$$ss^\dagger+tt^\dagger=1 \quad st'=ts'. \tag{37}$$

It is easy to see that if the conditions (37) are satisfied, S becomes a simplectic matrix, i.e., it leaves the form

$$F=\left\|\begin{matrix} 0 & 1 \\ -1 & 0 \end{matrix}\right\| \tag{38}$$

invariant in the sense that

$$SFS' = F. \tag{39}$$

It follows that the sets w_{-1k}, w_{-1*k} are obtained from the sets v_{-1k}, v_{-1*k} by a unitary simplectic transformation.

The calculation of the last paragraph shows that the role of vectors $v_{\omega k}$, $v_{\omega *k}$ for $\omega = -1$ is quite different from the role of the vectors $v_{\omega k}$, $v_{\omega *k}$ for complex ω. The fact that the same Eq. (24) holds for $\omega = -1$ and for complex ω is somewhat accidental.

It may be well to note at this point that the equation

$$Aw = \nu w \tag{40}$$

with complex ν does not imply that ν is one of the ω. In fact, (40) holds with $w = (\nu^{\frac{1}{2}})^* v_{1k}$ and an arbitrary ν.

5.

Lastly, we shall determine the number of free parameters in an antiunitary transformation which can be characterized by l invariant vectors; $2m$ vectors with the characteristic value -1; 2ρ different complex characteristic values with positive imaginary parts and their complex conjugates with multiplicities $c_1, c_2, \cdots, c_\rho$. These are then also the multiplicities of the corresponding conjugate complex characteristic values. Hence,

$$l + 2m + 2c_1 + 2c_2 + \cdots + 2c_\rho = n, \tag{41}$$

where n is the number of dimensions of the underlying Hilbert space which will be assumed to be finite dimensional in the present section.

The number of free parameters will be calculated by adding the free parameters necessary to characterize the complete orthonormal set v_{1k}, $v_{\omega k}$ and the ω, and subtracting the number of parameters contained in the transformations which alter the v but leave A unchanged. These were determined in the preceding section.

A complete orthonormal set in n dimensions can be characterized by $2n-1+(2n-3)+\cdots+3+1 = n^2$ parameters. The number of free parameters in the ω is just ρ. Hence, $n^2+\rho$ parameters are necessary to characterize the v and the ω.

A rotation in the l-dimensional space of the v_{1k} does not change A. The number of parameters of such a rotation is $\frac{1}{2}l(l-1)$. Similarly, a $2m$-dimensional unitary simplectic transformation remains free for the vectors $v_{-11}, \cdots, v_{-1m}, v_{-1*1}, \cdots, v_{-1*m}$. The number of parameters of such a transformation is $m(2m+1)$. Finally, an arbitrary unitary transformation of the vectors $v_{\omega 1}$, $v_{\omega 2}$, $\cdots$ leaves A also unchanged if the conjugate complex transformation is applied to the vectors $v_{\omega *1}$, $v_{\omega *2}$, $\cdots$. The number of parameters in such a transformation is just the square of the corresponding c. Hence, the total number of free parameters in the antiunitary transformation is

$$p = n^2 + \rho - \tfrac{1}{2}l(l-1) - m(2m+1) - \sum_1^\rho c_r^2$$

$$= n^2 - \tfrac{1}{2}l(l-1) - m(2m+1) - \sum_1^\rho (c_r^2 - 1). \tag{42}$$

For even n, the number of parameters is just n^2 if all the characteristic values are complex and simple. Two invariant vectors decrease the number of parameters by 1, two characteristic values -1 by 3, if a complex characteristic value is doubly degenerate (the same then holds for the conjugate complex characteristic value) the number of parameters is also decreased by three.

The number of free parameters is also n^2 if n is odd and there are $n-1$ simple complex characteristic values and one invariant vector. Multiplicities among the complex characteristic values and the presence of a characteristic value -1 (which is always at least double) reduce the number of free parameters as in the case of even n.

The fact that the number of parameters is n^2 in the general case could have been inferred from the possibility of representing an antiunitary transformation in the form (6), i.e., as the product of a unitary transformation and complex conjugation. The number of free parameters in an n-dimensional unitary transformation is just n^2. The decrease in the number of free parameters (by 3) caused by the presence of a single pair of characteristic values -1 is remarkable.

6.

The preceding results will now be formulated in the language of projection operators and thus extended to the case in which there is a continuous spectrum. However, the proofs, which are rather obvious, will be omitted.

Consider again the unitary operator $\Lambda = A^2$. If 1 and -1 belong to the point spectrum of Λ, denote the corresponding projection operators by E_1 and E_{-1}. The projection operator which belongs to an interval J of the unit circle in the complex plane will be denoted by E_J. All these projection operators are self-adjoint, commute with Λ and with each other; the product of two of them is equal to the projection operator which corresponds to the intersection of the domains to which the two factors correspond. Furthermore,

$$\Lambda E_1 = E_1 \quad \Lambda E_{-1} = -E_{-1} \quad \lim \Lambda E_J = \omega E_J, \tag{43}$$

where the lim in the last equation indicates that J is an infinitely narrow interval around ω. We define the antiunitary operators

$$A_1 = AE_1 \quad A_{-1} = AE_{-1} \quad A_J = AE_J, \tag{44}$$

then

$$A = A_1 + A_{-1} + \lim \sum A_J. \tag{45}$$

The lim again indicates that the intervals J are infinitely narrow; they cover all the unit circle with the exceptions of the points 1 and -1. The intervals J will be assumed to lie either entirely in the upper half-plane, or entirely in the lower half-plane. The interval J^* will be the conjugate complex of the interval J.

It is good to recall, for the rest of this discussion, that A^{-1} is also an antiunitary operator and is, in fact, given by

$$A^{-1}=\Lambda^{-1}A=A\Lambda^{-1}. \quad (46)$$

A transforms every projection operator into the projection operator which corresponds to the conjugate complex domain

$$AE_1A^{-1}=E_1 \quad AE_{-1}A^{-1}=E_{-1} \quad AE_JA^{-1}=E_{J^*}. \quad (47)$$

These equations can be given a variety of forms by combining them with (43) and (44). The most interesting of these forms gives the projection operators in terms of the A_J. Thus

$$A_1^2=AE_1AE_1=E_1A^2E_1=E_1\Lambda E_1=E_1^2=E_1. \quad (48)$$

Similarly,

$$A_{-1}^2=-E_{-1} \quad \lim A_{J^*}A_J=\omega E_J. \quad (49)$$

Whereas, if J and L do not overlap,

$$A_{L^*}A_J=0. \quad (50)$$

These equations form a substitute for the equations involving the characteristic vectors v of A. As an example, we show that v_{-1k} and Av_{-1k} are orthogonal or, in the present language, that $E_{-1}\varphi$ and $AE_{-1}\varphi$ are orthogonal for any φ

$$(E_{-1}\varphi,AE_{-1}\varphi)=(A^2E_{-1}\varphi,AE_{-1}\varphi)$$
$$=(-E_{-1}\varphi,AE_{-1}\varphi)=0. \quad (51)$$

The second form follows from the antiunitary nature of A, the third from (43).