THE CHARACTERIZATION OF QUANTUM-MECHANICAL OPERATORS

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1. *Introduction.* It is well known that the operators mainly employed in quantum theory are hermitian; it is less well known amongst physicists that they are required, in addition, to be self-adjoint. This is essential for the validity of the result known in quantum theory as the representation theorem and in the mathematical theory as the resolution of the identity. The purpose of this paper is to show that the self-adjoint operators can be characterized by a condition which is nearer to having a physical significance than those given in the literature.

We begin by explaining the distinction. A linear operator H with domain $\mathfrak{D}_H$ dense in a Hilbert space $\mathfrak{H}$ is said to be hermitian (or symmetric) if for any pair of elements f, g of its domain
$$(Hf, g) = (f, Hg). \tag{1}$$
The condition (1) is easily seen to be equivalent to the condition
$$(Hf, f) \text{ real for all } f \text{ in } \mathfrak{D}_H, \tag{1'}$$
and this has the clear physical meaning that the operator represents an observable with real expectation values.

If for an element g of $\mathfrak{H}$ there exists a unique g^* such that for every element f of the domain $\mathfrak{D}_T$ of an operator T
$$(Tf, g) = (f, g^*),$$
then g is said to be in the domain $\mathfrak{D}_{T^*}$ of the adjoint T^* of T, and $T^*g = g^*$.

For two operators A and B, we write $A \supset B$ if A is an extension of B, i.e. if the domain of A includes that of B, and the two operators have the same values in the common domain. With this notation, (1) can be written
$$H \subset H^*.$$
The requirement that an operator be self-adjoint is the stronger condition (3)
$$H = H^*. \tag{2}$$
The condition given by von Neumann (1, 2) is that the ranges of values of $Hf - if$ and of $Hf + if$ are $\mathfrak{H}$. Operators satisfying (1) and this condition are called hypermaximal by von Neumann; the term is equivalent to self-adjoint.

A hermitian operator is called *maximal* if there is no hermitian operator which is an extension of it. A self-adjoint operator is necessarily maximal, but the converse is not true.

It seems reasonable to confine our attention to maximal operators, in the physical theory, on the following grounds. If an operator R is an extension of S, and these represent observables **R** and **S**, then whenever **S** is measurable so is **R** and the values are the same, but **R** is measurable and meaningful in states where **S** is not. Confining

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ourselves to observables with as wide a range of definition as possible, we confine ourselves to the maximal operators.

We now come to the problem of characterizing self-adjoint among the maximal operators. In (5) I showed that such a characterization could be based on a consideration of the existence of solutions of the Schrödinger equation

$$H\psi(t) = \frac{1}{i}\frac{d\psi}{dt}, \tag{3}$$

with given initial conditions $\psi(0) = \phi$. If (3) has a solution for all values of t for any given $\psi \in \mathfrak{D}_H$, and H is hermitian, then H must be self-adjoint. If it has a solution only for positive values of t, or only for negative values of t, then H is maximal but not self-adjoint. This is the basis of the characterization of this article; but we shall attempt to put the condition in a different form, since the Schrödinger equation in physics is significant physically only if H is the Hamiltonian, and we wish to characterize all self-adjoint operators.

Our argument is based on the following concepts:

A *motion* of a dynamical system will mean a law which for values of t in some interval including $t = 0$ assigns to each initial state of the system ϕ a state $\psi(t)$ which depends linearly on ϕ, is continuous in t, and tends to ϕ as $t \to 0$.

An operator A is called a *constant of the motion* if for any $\phi \in \mathfrak{D}_A$, $\psi(t) \in \mathfrak{D}_A$ for all t in the interval, and $(A\psi(t), \psi(t))$ is constant.

If U_t is defined by $U_t\phi = \psi(t)$, then U_t is a linear operator with $\mathfrak{H}$ as domain. We shall assume that the transformation from a state at time t to that at time t' depends only on $t - t'$ (as is the case in any dynamical motion with Hamiltonian independent of time). In this case

$$U_t U_{t'} = U_{t+t'}, \tag{4}$$

whenever t, t' and $t + t'$ are in the interval for which U_t is defined. Moreover, $U_0 = I$.

In all the cases to be considered the identity will be a constant of the motion, as it must be in any physical case. This implies that

$$(U_t\phi, U_t\phi) = (\phi, \phi).$$

An operator satisfying this condition is called *isometric*. If, in addition, it has all $\mathfrak{H}$ as range, and so has U^* as inverse, it is *unitary*.

Our main result is the following:

THEOREM 1. *A maximal hermitian operator R is self-adjoint if and only if there is a motion defined throughout $(-\infty, \infty)$, such that*

(a) R and I are constants of the motion;

(b) any closed operator with domain dense in $\mathfrak{H}$ which is a constant of the motion commutes with R.

It is necessary to give the definitions of commutation to be used:

If A is a general operator and B a bounded operator, A is said to commute with B if $AB \supset BA$.

If R is a general symmetric operator, we require only the following: S does not commute with R if there exist f for which RSf and SRf are both defined but are not equal.

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For R self-adjoint, we say S commutes with R if it commutes with every projector in the resolution of the identity of R.

By way of illustration, consider the operator $i\,d/dx$ in $L^2(-\infty,\infty)$ which represents the momentum on an infinite line. It is possible for a particle to move with constant expectation value of the momentum and of its powers indefinitely on the line; consequently the momentum operator is self-adjoint in $L^2(-\infty,\infty)$. On the other hand, the operator $i\frac{d}{dx}$ in $L^2(0,\infty)$ is hermitian only if its domain is restricted to functions with $f(0)=0$; and it is then maximal, but not self-adjoint. This corresponds to the fact that on a half-line a particle cannot have an infinite past as well as an infinite future with constant expectation value of the momentum and all its powers. The same situation arises for the radial momentum in three dimensions, since the sign of the radial momentum of a particle must change when it passes through the origin (cf. (7), p. 151; (8), p. 143).

2. *Proof of the main theorem.* Let a motion satisfying the requirements of the theorem exist and be defined by the operators U_t, $-\infty<t<\infty$. I is a constant of the motion, so that the U are isometric. (4) holds for all t and t', hence the U_t form a group with $U_0=I$, and U_{-t} the inverse of U_t. The U_t are therefore a one-parameter group of unitary operators, whose structure is given by Stone's theorem (4).

By hypothesis, for any $f\in\mathfrak{D}_R$ and any t,

$$(RU_tf,U_tf)=(Rf,f),$$

whence we can deduce easily that for any pair $f,\,g\in\mathfrak{D}_R$

$$(RU_tf,U_tg)=(Rf,g)=(U_tRf,U_tg),$$

since U_t is unitary, so that RU_tf-U_tRf is orthogonal to U_tg for any $g\in\mathfrak{D}_R$, and so is zero, since U_t is unitary and the domain of R dense in $\mathfrak{H}$. Thus

$$U_tR=RU_t. \tag{5}$$

If R is maximal but not self-adjoint, there exists a one-parameter semi-group of isometric operators V_s defined for $s\geqslant 0$, having all $\mathfrak{H}$ as domain, satisfying

$$V_0=I,\quad V_sV_{s'}=V_{s+s'}\quad(s,s'\geqslant 0); \tag{6}$$

and either

$$\frac{dV_sf}{ds}=iRV_sf\quad(f\in\mathfrak{D}_R), \tag{7}$$

or the same equation with sign reversed (see (5)). We shall suppose that (7) holds.

We now show that for all t and all positive s

$$U_tV_s=V_sU \tag{8}$$

holds. In fact, for any $f\in\mathfrak{D}_R$, U_tf is in $\mathfrak{D}_R$ for all t, and

$$\frac{d}{ds}(V_sU_tf)=iRV_sU_tf \tag{9}$$

for all $s\geqslant 0$. On the other hand, for any g,

$$\begin{aligned}\frac{d}{ds}(U_tV_sf,g)&=\frac{d}{ds}(V_sf,U_{-t}g)\\&=i(RV_sf,U_{-t}g)=i(RU_tV_sf,g),\end{aligned}$$

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i.e. in the notation of (5), $$\frac{\delta}{\delta s} U_t V_s f = iR U_t V_s f. \tag{10}$$

Thus $U_t V_s f$ and $V_s U_t f$ are both solutions of the equation

$$\frac{\delta}{\delta s}\psi(s) = iR\psi(s), \quad \psi(0) = U_t f,$$

and since by the theory of (5) this equation has a unique solution, (8) follows, for all elements in $\mathfrak{D}_R$; the extension to all $\mathfrak{H}$ is immediate because of the continuity of the operators.

Now write $\mathfrak{R}_s$ for the range of V_s, and $\mathfrak{R}$ for the limit of $\mathfrak{R}_s$ as $s \to \infty$. If $f \in U_t \mathfrak{R}_s$, then $f = U_t V_s g$ for some g, and hence $f = V_s U_t g \in \mathfrak{R}_s$. Conversely, if $f \in \mathfrak{R}_s$,

$$f = V_s g = U_t V_s U_{-t} g \in U_t \mathfrak{R}_s,$$

so that $U_t \mathfrak{R}_s = \mathfrak{R}_s$. In particular, $U_t \mathfrak{R} = \mathfrak{R}$. Moreover, since U_t is unitary, any element orthogonal to $\mathfrak{R}_s$ is taken into an element orthogonal to $\mathfrak{R}_s$. Thus

$$U_t(\mathfrak{R}_s \ominus \mathfrak{R}_{s'}) = \mathfrak{R}_s \ominus \mathfrak{R}_{s'}, \tag{11}$$

when $0 \leqslant s < s' \leqslant \infty$.

R is self-adjoint and V_s unitary in $\mathfrak{R}$, and we need consider only the orthogonal complement of $\mathfrak{R}$; or, what comes to the same thing, we may suppose $\mathfrak{R}$ empty. In that case $\mathfrak{H}$ (or $\mathfrak{H} \ominus \mathfrak{R}$ in general) is (by (5)) the direct sum of a finite or countable set of mutually orthogonal infinite dimensional spaces $\mathfrak{M}_k$ ($k = 1, 2, \ldots, n$, where n is the deficiency index of R), each of which may be represented linearly and isometrically on $L^2(0, \infty)$, in such a way that if $\phi \in \mathfrak{H}$ is represented by the sequence $\{f_k(x)\}$ of functions of $L^2(0, \infty)$,

$$\| \phi \|^2 = \sum_{k=1}^{n} \int_0^\infty | f_k(x) |^2 dx,$$

and $$V_s \phi \to \{f_k(x-s)\},$$

where we take $f(x) = 0$ for $x < 0$.

From now on, elements of $\mathfrak{H}$ will be replaced by their representations as sequences of elements of $L^2(0, \infty)$, and the operations on these representations corresponding to R, U, V on the original elements will be denoted by the same letters as before. We need an expression for the form of U_t which is given by the following lemma†.

Any bounded linear operation T taking $L^2(0, a)$ into itself has the form

$$(Tf)(x) = \frac{d}{dx}\int_0^a k(x, y) f(y)\, dy,$$

where $k(x, y)$ is in $L^2(0, a)$ as a function of y for any x.

T^* exists and has all L^2 as domain. Put

$$g_x(y) = 1 \ \ (0 \leqslant y \leqslant x), \quad g_x(y) = 0 \ \text{ otherwise},$$

and $$(T^* g_x)(y) = \overline{k(x, y)}.$$

Then the identity $$(Tf, g_x) = (f, T^* g_x)$$

gives $$\int_0^x (Tf)(y)\, dy = \int_0^a k(x, y) f(y)\, dy,$$

† Due essentially to F. Riesz, *Math. Ann.* 67 (1910), 404.

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which is the result to be proved. With a slight modification of the proof the theorem can be extended to $L^2(-\infty, a)$.

Now if we put $$U_t\{f_k\} = \{g_k^t\},$$

then $g_k^t = \Sigma U_{kl}^t f_l$, where U_{kl}^t is a bounded transformation of $L^2(0,\infty)$ into itself, and hence, by the lemma,

$$g_k^t(x) = \Sigma \frac{d}{dx}\int_0^\infty K_{kl}^t(x,y)\, f_l(y)\, dy,$$

where $K(x,y)$ is in $L^2(0,\infty)$ for all x, and the differential coefficients exist in L^2. The commutation relations between the V's and the U's restrict the K's.

First, $U_t\{\mathfrak{R}_b \ominus \mathfrak{R}_a\} = \{\mathfrak{R}_b \ominus \mathfrak{R}_a\}$. In our representation, $\mathfrak{R}_a$ is the set of elements $\{f_k\}$ with $f_k(x) = 0$ for $x < a$, for all k. Denoting by K a generic K_{kl}^t we find that

$$\int_a^b \{K(x,y) - K(x',y)\} f(y)\, dy = 0,$$

if $x > x' > b$ or $a > x > x'$ for any f, a, b, and hence $K(x,y) = K(x',y)$ if y is not in (x,x').

Thus $$K(x,y) = K_1(y), \text{ for } x \geqslant y \quad \text{and} \quad K(x,y) = K_2(y), \text{ for } x < y,$$

and hence we get for U_t the form

$$U_t\{f_k\} = \{\Sigma u_{kl}(t,x)\, f_l(x)\}.$$

From this
$$U_t V_s\{f_k\} = \{\Sigma u_{kl}(t,x)\, f_l(x-s)\},$$
$$V_s U_t\{f_k\} = \{\Sigma u_{kl}(t,x-s)\, f_l(x-s)\},$$

and since these are always equal, u_{kl} cannot involve x,

$$U_t\{f_k\} = \{\Sigma u_{kl}(t)\, f_l\}.$$

The U_t therefore have constant values over each of the spaces $\mathfrak{M}_k$, and so commute with any operator which takes each of these manifolds into itself: for example, the operator

$$G\{f_k\} = \{x f_k(x)\}$$

is an operator which commutes with U_t for all t, but does not commute with R (or with V_s).

We have shown that if R is not self-adjoint there must exist bounded operators which are constants of the motion but do not commute with R. Hence if a motion of the type considered exists, R must be self-adjoint.

On the other hand, if R is self-adjoint, the operators V_s defined as above by (7) are defined for all s, and give a motion satisfying the requirements of the theorem. For R is clearly a constant of this motion; and if S is a bounded operator such that $SR \subset RS$ (our definition of commutation), then, for any $f \in \mathfrak{D}_R$,

$$\frac{d}{dt} SV_t f = S\left(\frac{d}{dt} V_t f\right) = iSRV_t f,$$

by the boundedness of S, and hence by the commutativity

$$\frac{d}{dt} SV_t f = iRSV_t f,$$

whence
$$\frac{d}{dt}(SV_t f, V_t f) = i(RSV_t f, V_t f)\,(SV_t f, iRV_t f)$$
$$= 0.$$

Hence $(SV_t f, V_t f)$ is constant in t for any f, and by the boundedness of S and V this follows for all f.

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Conversely, suppose that S is a bounded operator such that (SV_tf, V_tf) is constant for any $f \in \mathfrak{H}$. Then, if $f, g \in \mathfrak{D}_R$,

$$0 = \frac{d}{dt}(SV_tf, V_tg) = \left(S\frac{d}{dt}V_tf, V_tg\right) + \left(SV_tf, \frac{d}{dt}V_tg\right)$$
$$= i(SRV_tf, V_tg) + (SV_tf, iRV_tg),$$

because of the boundedness of S. It follows that $SV_tf \in \mathfrak{D}_R$ and that $RSV_tf = SRV_tf$ when $f \in \mathfrak{D}_R$. On taking $t = 0$, this gives $SR \subset RS$.

If S is unbounded, we have (SV_tf, V_tg) constant for any $f, g \in \mathfrak{D}_S$, and consequently by continuity for any $f \in \mathfrak{D}_S$ and any g. Taking $g \in \mathfrak{D}_{S^*}$, we have

$$(SV_tf, g) = (V_tf, S^*g) = \int_{-\infty}^{\infty} e^{i\lambda t} d(E_\lambda f, S^*g),$$

and

$$(V_tSf, g) = \int_{-\infty}^{\infty} e^{i\lambda t} d(E_\lambda Sf, g),$$

where E_λ is the resolution of the identity of R. Since these expressions are equal for all t, and the integrands are zero for $\lambda = -\infty$,

$$(E_\lambda Sf, g) = (E_\lambda f, S^*g)$$

for all λ, all $f \in \mathfrak{D}_S$ and $g \in \mathfrak{D}_{S^*}$. Thus $E_\lambda f \in \mathfrak{D}_{S^{**}}$ and $E_\lambda Sf = S^{**}E_\lambda f = SE_\lambda f$ if S is closed. The converse, that if S is closed and commutes with the projectors E_λ then it is a constant of the motion, follows in the same way.

Thus for a self-adjoint operator the motion defined by (7) is one which fulfils the requirements of the theorem.

It may be asked whether a sort of converse of Theorem 1 would hold: that if R is a self-adjoint operator, and V_s a motion defined in $(0, \infty)$ for which R and the operators which commute with it are the set of constants of the motion, then the set V_s can be extended to a set over $(-\infty, \infty)$ with the same property. This is not necessarily true, as can be seen by taking $R = I$. However, the analysis by which Theorem 1 was proved (using (6)) shows that if the statement fails, so that there is a one-parameter semi-group of isometric non-unitary operators commuting with R, then R is infinitely degenerate. In fact, if V_s is represented in terms of its invariant manifolds $\mathfrak{M}_k$ as in Theorem 1, R must have the form

$$R\{f_i\} = \{\Sigma c_{il} f_l\},$$

where $\{c_{il}\}$ is a hermitian matrix; and any manifold in its spectrum is a Hilbert space.

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