ON THE HERMITEAN OPERATORS IN QUANTUM MECHANICS

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ABSTRACT.

The main purpose of this paper is, after making some necessary preliminaries on the theory of linear differential operators in one real variable, to obtain the explicit condition that such an operator of any order be a Hermitean operator, and as application of the result point out various quantum-mechanical instances.

In Quantum Mechanics, expressions like pqp , qp^2 , p^2q are different from each other, the first being a Hermitean operator but the remaining two being not ⁽¹⁾. The second is already in usual differential form (polynomial in $p = \frac{h}{2\pi i} \frac{d}{dq}$ with functions of q as left-hand coefficients), and the two others are reducible to usual differential forms by the aid of the commutation rule $pq - qp = \frac{h}{2\pi i} 1$, thus

$$pqp = \left(qp + \frac{h}{2\pi i} 1 \right) p = qp^2 + \frac{h}{2\pi i} p,$$

$$p^2q = p \left(qp + \frac{h}{2\pi i} 1 \right) = \left(qp + \frac{h}{2\pi i} 1 \right) p + \frac{h}{2\pi i} p = qp^2 + \frac{h}{\pi i} p.$$

Now, according to Schroedinger, every quantum-mechanical problem is ultimately reduced to a question concerning a Hermitean operator in one variable. It is therefore useful to find the condition which must be satisfied in order that the general *linear differential operator*

$$a_n \frac{d^n}{dx^n} + a_{n-1} \frac{d^{n-1}}{dx^{n-1}} + \dots + a_1 \frac{d}{dx} + a_0$$

in one (real) variable x be Hermitean. Here the a 's are functions of x which we suppose to have derivatives up to a sufficiently high order in a certain given

I. E. T. Whittaker, "On Hamilton's principal function in quantum mechanics," *Proc. Roy. Soc. Edin. A* 61 (1941), 4.

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interval of x . The leading coefficient a_n is assumed different from zero in this interval, and the differential operator is said to be of *order* n . We shall first make some preparation on the theory of such operators.

1. Addition and Multiplication of Differential Operators.

Consider two operators

$$A = \sum_{r=0}^n a_r \frac{d^r}{dx^r}, \quad B = \sum_{s=0}^m b_s \frac{d^s}{dx^s}$$

of orders n, m respectively. Their *sum* or *difference* $A \pm B$ is defined by

$$A \pm B = \sum \left(a_t \pm b_t \right) \frac{d^t}{dx^t}$$

which is an operator of order $= \max(n, m)$ if $m \neq n$, or $\leq n$ if $m = n$.

To define the *product* AB we assume that the b 's have derivatives up to order n . Then by definition

$$\begin{aligned} AB &= \sum_{r=0}^n a_r \frac{d^r}{dx^r} \left(\sum_{s=0}^m b_s \frac{d^s}{dx^s} \right) \\ &= \sum_{r=0}^n \sum_{s=0}^m a_r \sum_{\lambda=0}^r \binom{r}{\lambda} b_s \frac{d^{s+\lambda}}{dx^{s+\lambda}} \\ &= \sum_{t=0}^{n+m} p_t \frac{d^t}{dx^t} \end{aligned}$$

where

$$p_t = \sum_{s=0}^t \sum_{r=t-s}^n \binom{r}{t-s} a_r b_s^{(r+s-t)} \quad (t=0, 1, \dots, n+m). \quad (1)$$

In particular we find $p_{n+m} = a_n b_m$, thus BA is an operator of order $n+m$.

If the a 's are assumed m times differentiable, the product AB also exists but is in general not equal to BA .

It can be verified, by the aid of (1) that for three operators A, B, C , the associative law

$$(AB)C = A(BC)$$

holds, the differentiability of the coefficients of B and C being assumed. It is easy to see that there also hold the distributive laws

$$(A \pm B)C = AC \pm BC, \quad C(A \pm B) = CA \pm CB.$$

2. The Transpose of an Operator.

To every operator A there corresponds a unique operator $\tilde{A}$ such that

$$vAu = u\tilde{A}v + \text{exact derivative.} \quad (2)$$

To prove this, let

$$A = a_n \frac{d^n}{dx^n} + a_{n-1} \frac{d^{n-1}}{dx^{n-1}} + \dots + a_1 \frac{d}{dx} + a_0$$

and write $va_i = a_i$ ($i=0, 1, \dots, n$) for brevity. We have

$$\begin{aligned} vAu &= a_n u^{(n)} + a_{n-1} u^{(n-1)} + \dots + a_1 u' + a_0 u \\ &= [a_n u^{(n-1)}]' + (a_{n-1} - a_n') u^{(n-1)} + a_{n-2} u^{(n-2)} + \dots \\ &= [a_n u^{(n-1)} + (a_{n-1} - a_n') u^{(n-2)}]' + (a_{n-2} - a_{n-1}' + a_n'') u^{(n-2)} \\ &\quad + a_{n-3} u^{(n-3)} + \dots \\ &= \dots \\ &= [a_n u^{(n-1)} + \{a_{n-1} - a_n'\} u^{(n-2)} + \{a_{n-2} - a_{n-1}' + a_n''\} u^{(n-3)} + \dots \\ &\quad + \{a_2 - a_3' + a_4'' - \dots + (-1)^{n-2} a_n^{(n-2)}\} u' \\ &\quad + \{a_1 - a_2' + a_3'' - \dots + (-1)^{n-1} a_n^{(n-1)}\} u]' + wu \end{aligned}$$

where

$$\begin{aligned} w &= \sum_{r=0}^n (-1)^r a_r^{(r)} = \sum_{r=0}^n (-1)^r (v a_r)^{(r)} \\ &= \sum_{i=0}^n \tilde{a}_i v^{(i)} = \tilde{A}v \end{aligned}$$

where

$$\tilde{a}_i = \sum_{r=i}^n (-1)^r \binom{r}{i} a_r^{(r-i)} \quad (i=0,1,\dots,n) \quad (3)$$

and
$$\tilde{A} = \tilde{a}_n \frac{d^n}{dx^n} + \tilde{a}_{n-1} \frac{d^{n-1}}{dx^{n-1}} + \dots + \tilde{a}_1 \frac{d}{dx} + \tilde{a}_0.$$

We have thus established an identity of the form (2) where $\tilde{A}$ is an operator whose coefficients are given by (3). It is seen that $\tilde{A}$ is uniquely determined.

From (3) we find in particular

$$\tilde{a}_n = (-1)^n a_n. \quad (4)$$

Hence $\tilde{A}$ has the same order n as A .

We call $\tilde{A}$ the *transpose* of A . It is clear from (2) that, conversely, A is the *transpose* of $\tilde{A}$. This fact is symbolically expressed by

$$\tilde{\tilde{A}} = A. \quad (5)$$

In terms of coefficients, (5) is equivalent to

$$\tilde{\tilde{a}}_i = a_i \quad (i=0,1,\dots,n) \quad (6)$$

where, analogous to (3),

$$\tilde{\tilde{a}}_i = \sum_{r=i}^n (-1)^r \binom{r}{i} \tilde{a}_r^{(r-i)} \quad (i=0,1,\dots,n). \quad (7)$$

We may also prove (6) directly by substituting (3) into (7).

By (7), we may write (6) in the form

$$a_i = \sum_{r=i}^n (-1)^r \binom{r}{i} \tilde{a}_r^{(r-i)} \quad (i=0,1,\dots,n). \quad (8)$$

This, as we see, is merely (3) with the a 's and $\tilde{a}$'s interchanged. The reciprocal relationship between A and $\tilde{A}$ is thus confirmed.

Note. As in the theory of differential equations one might call $\tilde{A}$ the *adjoint* of A . However, we prefer the language used in the theory of matrices, calling $\tilde{A}$ the transpose of A and reserving the word adjoint for another purpose.

3. The Bilinear Form Corresponding to an Operator.

Let the exact derivative in (2) be denoted by φ' . Then, omitting an unimportant additive constant, φ is, as we have seen above, given by

$$\begin{aligned} \varphi &= \sum_{i=0}^{n-1} \{a_{i+1} - a''_{i+2} + a''_{i+3} - \dots + (-1)^{n-i-1} a_n^{(n-i-1)}\} u^{(i)} \\ &= \sum_{i=0}^{n-1} u^{(i)} \sum_{r=0}^{n-i-1} (-1)^r a_{i+1+r}^{(r)} = \sum_{i=0}^{n-1} u^{(i)} \sum_{r=0}^{n-i-1} (-1)^r (v a_{i+r+1})^{(r)} \\ &= \sum_{i=0}^{n-1} u^{(i)} \sum_{k=0}^{n-1} v^{(k)} \sum_{r=k}^{n-i-1} (-1)^r \binom{r}{k} a_{i+r+1}^{(r-k)} \end{aligned}$$

which is a bilinear form in the two sets of variables

$$u, \quad u', \quad u'', \quad \dots, \quad u^{(n-1)};$$

$$v, \quad v', \quad v'', \quad \dots, \quad v^{(n-1)}.$$

This bilinear form may be written

$$\varphi(u, v) = \sum_{i,k=0}^{n-1} a_{ik} u^{(i)} v^{(k)} \quad (9)$$

where

$$a_{ik} = \sum_{r=k}^{n-i-1} (-1)^r \binom{r}{k} a_{i+r+1}^{(r-k)} \quad (i, k=0, 1, \dots, n-1). \quad (10)$$

When $n-i-1 < k$, we have $a_{ik}=0$ since the summation on the right of the above formula is then empty. Hence the matrix

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & \dots \\ a_{10} & a_{11} & a_{12} & \dots \\ a_{20} & a_{21} & a_{22} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (11)$$

has zero elements below the non-principal diagonal, it being *triangular* matrix. The elements on this non-principal diagonal are obtained by setting $n-i-1=k$ in (10), giving

$$a_{n-1-k,k} = (-1)^k a_n \quad (k=0, 1, \dots, n-1). \quad (12)$$

It follows that

$$\det (a_{ik}) = a_n^n \quad (13)$$

and therefore the bilinear form (9) is non-singular.

We call $\mathcal{P}(u,v)$ the bilinear form corresponding to the operator A . The relation between $\mathcal{P}(u,v)$, A and $\tilde{A}$ is expressed by (2), which may now be written

$$vAu - u\tilde{A}v = \frac{d}{dx} \mathcal{P}(u,v). \quad (14)$$

It may be observed that in the theory of transposed operators as developed above, it suffices to assume that a_r possesses derivatives up to order r .

4. Transposition of Products.

Consider two operators A and B , and suppose that their coefficients have derivatives up to sufficiently high orders. We now show that the transpose of the product AB is equal to the product of the transposes of A and B taken in reversed order:

$$\overline{BA} = \tilde{B} \tilde{A}. \quad (15)$$

In fact, we have

$$\begin{aligned} v(AB)u &= vA\xi & (\xi &= Bu) \\ &= \xi \tilde{A} v + * & (* &= \text{exact derivative}) \\ &= \xi \eta + * & (\eta &= \tilde{A} v) \\ &= \eta Bu + * \\ &= u \tilde{B} \eta + * + * \\ &= u (\tilde{B} \tilde{A}) v + * \end{aligned}$$

whence the transpose of AB is equal to $\tilde{B}\tilde{A}$. Since the transpose is unique, (15) is proved.

We may also verify (15) directly by making use of (1) and (3).

5. The Conjugate of an Operator.

We assume for the sake of generality that the coefficients of the operators are complex functions of the real variable x . Then to every operator $A = \sum a_r \frac{d^r}{dx^r}$ there corresponds a *conjugate operator* $\bar{A} = \sum \bar{a}_r \frac{d^r}{dx^r}$, where $\bar{a}$ denotes the conjugate complex of a . It is clear that $\bar{A}$ has the same order as A , and that the following rules hold:

$$\overline{\bar{A}} = A. \quad (16)$$

$$\overline{AB} = \bar{A} \bar{B}. \quad (17)$$

6. The Adjoint of an Operator.

It is evident that, A being any operator, the two operators $\bar{A}$ and $\tilde{A}$ are equal to each other. We shall write

$$A^* = \overline{\overline{A}} = \overline{\overline{\overline{A}}}$$

and call A^* the *adjoint* of A . Clearly, the order of A^* equals that of A , so that if A is of the form

$$A = \sum_{i=0}^n a_i \frac{d^i}{dx^i},$$

then A^* is of the same form

$$A^* = \sum_{i=0}^n a_i^* \frac{d^i}{dx^i},$$

where, by (3),

$$a_i^* = \sum_{r=i}^n (-1)^r \binom{r}{i} \bar{a}_r^{(r-i)} \quad (i=0,1,\dots,n). \quad (18)$$

In particular, we have

$$a_n^* = (-1)^n \bar{a}_n. \quad (19)$$

We find, by (5) and (16),

$$A^{**} = A, \quad (20)$$

and by (15) and (17),

$$(AB)^* = B^* A^*. \quad (21)$$

7. Hermitean Operators.

An operator $A = \sum_{i=0}^n a_i \frac{d^i}{dx^i}$, of order n , is said to be *self-adjoint*, or

Hermitean, if $A^* = A$. The condition for this is $a_i^* = a_i$ ($i=0,1,\dots,n$) or, by (18),

$$a_i = \sum_{r=i}^n (-1)^r \binom{r}{i} \bar{a}_r^{(r-i)} \quad (i=0,1,\dots,n). \quad (22)$$

We may write this in the equivalent form

$$\bar{a}_i = \sum_{r=i}^n (-1)^r \binom{r}{i} a_r^{(r-i)} \quad (i=0,1,\dots,n). \quad (23)$$

In particular, we have (24)

$$\bar{a}_n = (-1)^n a_n.$$

Thus, a_n must be real if n is even, and purely imaginary if n is odd

Note. An operator A is said to be *symmetric* if $\tilde{A} = A$. One might develop a theory of symmetric operators along parallel lines as the theory of Hermitean operators. However, the latter theory is of deeper significance than the former for many purposes. The two theories become identical when (and only when) the operators have real coefficients.

8. Hermitean Operators of Order Zero.

For $n=0$, (23) consists of the single equation (24) which now reads $\bar{a}_0 = a_0$, i.e., a_0 is real. Hence, a function $a_0 = f(x)$ regarded as an operator of order zero is Hermitean if and only if it is real.

For example, x itself is a Hermitean operator, the *coordinate operator* in Quantum Mechanics.

9. Hermitean Operators of Order One.

For $n=1$, (23) implies that a_1 and a_0 are of the form

$$a_1 = i f(x), \quad a_0 = g(x) + i f'(x)/2, \quad (25)$$

where $f(x)$ and $g(x)$ denote real functions of x . Hence an operator of order one is Hermitean if and only if it is of the form

$$i f(x) \frac{d}{dx} + g(x) + \frac{i}{2} f'(x). \quad (26)$$

For example, taking $f = -\hbar/2\pi$ and $g=0$, where $\hbar$ denotes Planck's constant, we obtain the Hermitean operator $\frac{\hbar}{2\pi i} \frac{d}{dx}$, the *momentum operator* in Quantum Mechanics.

10. *Hermitean Operators of Order Two.*

For $n=2$, we find from (23) that a_2 , a_1 and a_0 are of the form

$$a_2=f(x), \quad a_1=f'(x)+ig(x), \quad a_0=k(x)+ig'(x)/2. \quad (27)$$

where $f(x)$, $g(x)$ and $k(x)$ denote real functions of x . Hence an operator of order two is Hermitean if and only if it is of the form

$$f(x) \frac{d^2}{dx^2} + \left\{ f'(x) + ig(x) \right\} \frac{d}{dx} + \left\{ k(x) + \frac{i}{2} g'(x) \right\}. \quad (28)$$

Example 1. Taking $f = -\hbar^2/8\pi^2\mu$ and $g=0$, where μ is a real constant, we have the Hermitean operator

$$-\frac{\hbar^2}{8\pi^2\mu} \frac{d^2}{dx^2} + k(x)$$

which, when $\mu > 0$, is the Hamiltonian operator for the quantum mechanical problem of a particle of mass μ and potential energy $k(x)$. In particular, for the *harmonic oscillator*, we set $k(x) = 2\pi^2\mu v^2 x^2$ where v is the classical frequency of the oscillator.

Example 2. Taking $f(x) = 1-x^2$, $g(x) = 0$, and $k(x) = l(l+1) - m^2/(1-x^2)$, where l and m are real constants, we have the Hermitean operator

$$(1-x^2) \frac{d}{dx^2} - 2x \frac{d}{dx} + l(l+1) - \frac{m^2}{1-x^2}$$

whose eigenfunctions are the (associated) *spherical harmonics* (*Legendre's functions*) of "degree" l and "order" m , which characterise the quantum states of the *rotator* of azimuthal quantum number l and magnetic quantum number m .

Example 3. Taking $f(x) = x^2$, $g(x) = 0$, and the following $k(x)$, we have the Hermitean operator

$$\frac{d}{dx} \left(x^2 \frac{d}{dx} \right) + \left\{ \frac{8\pi^2\mu}{\hbar^2} (Ex^2 + Ze^2x) - l(l+1) \right\}$$

for the *radial function* of the *hydrogen atom* ($Z=1$) at the energy level E .

Example 4. Taking $f(x) = \sin^2 x$, $g(x) = 0$, and a suitable $h(x)$, we have the Hermitean operator

$$\frac{d}{dx} \left(\sin^2 x \frac{d}{dx} \right) + \left\{ \frac{8\pi^2 \mu a^2}{h^2} \left(E \sin^2 x + Ze^2 \frac{\sin 2x}{2a} \right) - l(l+1) \right\}$$

for the *Kepler problem in spherical space* (2).

Example 5. The following operators

$$(1-x^2) \frac{d^2}{dx^2} - x \frac{d}{dx} + n^2 \quad (\text{Tscheytscheff})$$

$$\frac{d^2}{dx^2} - 2x \frac{d}{dx} + 2n \quad (\text{Hermite})$$

$$(1-x^2) \frac{d^2}{dx^2} - (1+2x) \frac{d}{dx} + n(n+1) \quad (\text{Hermite})$$

$$x \frac{d^2}{dx^2} + (1-x) \frac{d}{dx} + n \quad (\text{Laguerre})$$

are not Hermitean operators, since they are not of the form (27).

Example 6. The hypergeometric operator

$$x(1-x) \frac{d^2}{dx^2} + \{ \gamma - (\alpha + \beta + 1)x \} \frac{d}{dx} - \alpha\beta$$

is Hermitean if and only if

$$\text{either } \begin{cases} \alpha = \alpha_1 + i\alpha_2 \\ \beta = 1 - \alpha_1 - i \frac{3 - 2\alpha_1}{1 + 2\alpha_1} \alpha_2 \\ \gamma = 1 + i\gamma_2 \end{cases} \quad \text{or } \begin{cases} \alpha = -\frac{1}{2} \\ \beta = \frac{3}{2} + i\beta_2 \\ \gamma = 1 + i\gamma_2 \end{cases}$$

where the new letters on the right denote arbitrary real constants ($\alpha_1 \neq -\frac{1}{2}$ in the first form).

(2) H. C. Lee, "On the factorisation method for quantum-mechanical eigenvalue problems," *Chinese J. Phys.* 5 (1944), 99.

11. *Hermitean Operators of Higher Orders.*

For $n > 2$, there is no difficulty to determine similarly from (23) the expressions of $a_n, a_{n-1}, \dots, a_1, a_0$ in terms of arbitrary real functions, so as to obtain a general form of a Hermitean operator of order n . But, as Schrodinger's equation is of the second order, a knowledge of the cases $n \leq 2$ is already sufficient for the practical quantum-mechanical problems. However, as in Classical Mechanics, where the Hamiltonian can be no longer quadratic in the momenta after contact transformations, so in Quantum Mechanics too, every Hermitean operator of every order n can be thought of as defining a quantum mechanical problem, at least theoretically.

12. *Monomial Hermitean Operators.*

Putting $a_0 = a_1 = \dots = a_{n-1} = 0$ in (23) we find, in addition to (24), that a_n must be a constant. Hence a monomial operator $a \frac{d^n}{dx^n}$ of order n is Hermitean if and only if its coefficient a is a real constant when n is even, and a purely imaginary constant when n is odd.

13. *Sums and Products of Hermitean Operators.*

Let A and B be two Hermitean operators: $A^* = A, B^* = B$. Since it is clear that $(A \pm B)^* = A^* \pm B^*$, we have now $(A \pm B)^* = A \pm B$. Hence the sum and difference of two Hermitean operators are also Hermitean operators.

By (21), we have now $(AB)^* = BA$. Hence the product of two Hermitean operators is a Hermitean operator if and only if the two operators commute with each other.

Example 1. The quantum-mechanical operator $-\frac{h^2}{8\pi^2\mu} \frac{d^2}{dx^2} + k(x)$, mentioned in §10, Ex. 1, is a sum of two Hermitean operators and therefore is itself a Hermitean operator.

Example 2. Forming the square of the Hermitean operator in §10, Ex. 2, we obtain the Hermitean operator of order four:

$$\left[(1-x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx} + k \right]^2 = (1-x^2)^2 \frac{d^4}{dx^4} - 8x(1-x^2) \frac{d^3}{dx^3} + \dots$$

$$+ \{(k-6) - (k-14)x^2\} \frac{d^2}{dx^2} - 2(k-2)x \frac{d}{dx} \\ + \{(1-x^2)k' - 2xk' + k^2\}.$$

14. *The Bilinear Form Corresponding to a Hermitean Operator.*

The bilinear form corresponding to a Hermitean operator has, but for the factor i , a Hermitean matrix, that is to say, under the condition (23), (11) is a Hermitean skew-symmetric matrix:

$$\bar{a}_{ki} = -a_{ik} \quad (29)$$

To prove this, we have by (10)

$$a_{ki} = \sum_{s=i}^{n-k-1} (-1)^s \binom{s}{i} a_{k+s+1}^{(s-i)},$$

so that

$$\begin{aligned} \bar{a}_{ki} &= \sum_{s=i}^{n-k-1} (-1)^s \binom{s}{i} \bar{a}_{k+s+1}^{(s-i)} \\ &= \sum_{s=i}^{n-k-1} (-1)^s \binom{s}{i} \left\{ \sum_{t=k+s+1}^n (-1)^t \binom{t}{k+s+1} a_t^{(t-k-s-1)} \right\}^{(s-i)} \text{ by (23)} \\ &= \sum_{s=i}^{n-k-1} (-1)^s \binom{s}{i} \left\{ \sum_{t=k+s+1}^n (-1)^t \binom{t}{k+s+1} a_t^{(t-i-k-1)} \right\} \\ &= \sum_{t=i+k+1}^n (-1)^t \left\{ \sum_{s=i}^{t-k-1} (-1)^s \binom{s}{i} \binom{t}{k+s+1} \right\} a_t^{(t-i-k-1)} \end{aligned}$$

Now it can be shown (see Note below) that

$$\sum_{s=i}^{t-k-1} (-1)^s \binom{s}{i} \binom{t}{k+s+1} = (-1)^i \binom{t-i-1}{k}, \quad (30)$$

whence

$$\begin{aligned}\bar{a}_{ki} &= \sum_{t=i+k+1}^n (-1)^t (-1)^i \binom{t-i-1}{k} a_t^{(t-i-k-1)} \\ &= \sum_{r=k}^{n-i-1} (-1)^{r+1} \binom{r}{k} a_{i+r+1}^{(r-k)}\end{aligned}$$

and therefore, in view of (10), (29) is established.

Note. To prove (30) we remark that for $|\theta| < 1$ we have

$$(1+\theta)^{-i-1} = (-1)^i \theta^{-i} \sum_{s=i}^{\infty} (-1)^s \binom{s}{i} \theta^s.$$

Hence

$$\begin{aligned}(1+\theta)^{t-i-1} &= (1+\theta)^{-i-1} (1+\theta)^t \\ &= (-1)^i \theta^{-i} \left\{ \sum_{s=i}^{\infty} (-1)^s \binom{s}{i} \theta^s \right\} \left\{ \sum_{\sigma=0}^{\infty} \binom{t}{\sigma} \theta^{\sigma} \right\},\end{aligned}$$

so that by comparing the coefficients of $\theta^{t-i-k-1}$ we obtain

$$\binom{t-i-1}{t-i-k-1} = (-1)^i \sum_{s=i}^{t-k-1} (-1)^s \binom{s}{i} \binom{t}{t-k-1-s}$$

which is (30).