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About the Relation $[X,P] = i$

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Abstract

By means of an example it is illustrated that the usual canonical commutation relation is not equivalent to the canonical commutation relation in the Weyl form. The example is also used to show that several well-known operator identities, in the author's opinion, are false because they were derived by formal power series expansions.

The canonical commutation relation (CR) between position and momentum,

$$[X,P] = i \tag{1.1}$$

is of fundamental importance in quantum mechanics. One would like to have the result that CR (1.1) uniquely defines a pair of self-adjoint operators in a Hilbert space. However, CR (1.1) yields the usual Schrödinger position and momentum operators, which are defined in the space $L^2(-\infty, \infty)$ of square-integrable functions on the real line, as its unique solution only if rather technical additional assumptions are made, which have no obvious physical significance. [See Chapter IV in Putman (1967) and references there as well as Jauch (1968).]

On the other hand, the so-called Weyl form of CR(1),

$$e^{iaP}e^{ibX} = e^{iab}e^{ibX}e^{iaP} \qquad (-\infty < a, b < \infty) \tag{1.2}$$

has a unique irreducible self-adjoint solution (up to unitary equivalence), namely the Schrödinger operators mentioned above (von Neumann, 1931). CR (1.2) can be proved from CR (1.1) by using a formal power series expansion. The inequivalence of CR (1.1) and CR (1.2) is due to the fact that formal power series in general do not lead to correct results if unbounded operators

† It can be shown that two operators X and P satisfying CR(1) cannot both be bounded. See Theorem 1.2.1 in Putnam (1967).

are involved. In this note, I would like to illustrate by means of a concrete example of a pair of self-adjoint operators satisfying CR (1.1) but not CR (1.2) that the uniqueness problem of the two relations (1.1) and (1.2) is quite different. The example will emerge by examining a well-known textbook formula involving the exponentiation of a self-adjoint operator. This formula, as well as similar ones, turns out to be wrong in general because it, as CR (1.2), is derived by formal power series expansion. The example also illuminates why formal power series expansions of functions of unbounded operators are unreliable.

By formal power series expansion, one can derive the operator relation

$$e^{iaP}X\,e^{-iaP} = X + ia/1!\,[P, X] + (ia)^2/2!\,[P, [P, X]] + \cdots \tag{1.3}$$

which is often quoted in textbooks either with the explicit comment that it is valid for any two operators X and P (Lurié, 1968) or at least without stating any restrictions on its validity (Messiah, 1966). We will now exhibit an important operator pair X, P which does not satisfy formula (1.3). To find it we note that formula (1.3) implies that X is unbounded if X and P satisfy CR (1.1). The reason is the following. For a solution of CR (1.1), formula (1.3) reduces to

$$e^{iaP}X\,e^{-iaP} = X + a \tag{1.4}$$

Let us assume that X is bounded. Since, according to spectral theory (Yosida, 1971), e^{iaP} for self-adjoint P and arbitrary real a is unitary and therefore also bounded, equation (1.4) must be a valid operator identity when applied to any vector ψ in the space. Thus, together with the unitarity of e^{iaP}, equation (1.4) implies

$$(e^{-iaP}\psi, X\,e^{-iaP}\psi) = (\psi, X\psi) + a(\psi, \psi) \tag{1.5}$$

Thus, given an arbitrary state ψ, for which X has the expectation value $(\psi, X\psi)$, we can always find another state, $e^{-iaP}\psi$, for which X has as large or as small an expectation value as we like. We just need to choose a appropriately. This is a contradiction, and therefore X must be unbounded.

This result agrees with the familiar situation in which X and P are the usual Schrödinger position and momentum operators, which are both unbounded. Indeed, equation (1.4) is valid in this case and can be derived easily from the fact that e^{-iaP} is the translation operator in configuration space: $e^{-iaP}\psi(x) = \psi(x - a)$.† However, the result also suggests that in order to find an example for which equations (1.3) or (1.4) cannot be valid operator identities we should look for a solution to CR(1) with a bounded X. Such a solution is considered next.

Let X and P be operators satisfying CR (1.1) in the Hilbert space $L^2(c, d)$ of square-integrable functions of the variable x in the finite interval $[c, d]$. Both X and P are self-adjoint in this space if X is the multiplication by x, with domain equal to the entire space $L^2(c, d)$, and P is the differentiation operator

† A rigorous proof involving the Fourier transform is outlined in Section 4.2 in Putnam (1967).

$-id/dx$ with a domain consisting of the differentiable functions which are periodic in $[c, d]$, 'periodic' meaning here that $f(c) = f(d)$.† The operator X is bounded below and above by c and d while P is unbounded, which is related to the fact that the domain of P is a genuine subset of the space. These operators X and P therefore constitute an example for which equations (1.3) or (1.4) cannot be valid operator identities. The reader has probably already realized that this X and P and the space $L^2(c, d)$ are widely used in physics. If $[c, d]$ is the interval $[0, 2\pi]$, then X is an angular variable and P is the corresponding angular momentum component. If the interval $[c, d]$ is 'large', it constitutes the famous (one-dimensional, in this case) box in which we so often enclose systems.

To demonstrate that in fact equations (1.3) or (1.4) are not valid operator identities, say for the X and P in $L^2(0, 2\pi)$, let us calculate the expectation value of both sides of equation (1.4) for an eigenstate $f_m = 1/(2\pi)^{1/2} e^{imx}$ of P corresponding to the eigenvalue m. If equation (1.4) were an operator identity, it should clearly be applicable to f_m since all operators in (1.4) are bounded. The expectation value of the left-hand side of equation (1.4) equals

$$\begin{aligned}(f_m, e^{iaP} X\, e^{-iaP} f_m) &= (e^{-iaP} f_m, X\, e^{-iaP} f_m)\\ &= (e^{-iam} f_m, X\, e^{-iam} f_m)\\ &= (f_m, Xf_m)\end{aligned} \tag{1.6}$$

while that of the right-hand equals

$$(f_m, (X + a) f_m) = (f_m, Xf_m) + a \tag{1.7}$$

Since expressions (1.6) and (1.7) are not equal, relations (1.3) or (1.4) are shown to be invalid for the present X and P.

For the present X and P, relation (1.4) is valid when applied to any function $\psi(x)$ whose support lies entirely within $[0, 2\pi]$ as long as a is restricted so that translation by a does not carry the support of the considered function beyond 0 or 2π. This is so because for such a $\psi(x)$, with a restricted as indicated, $\psi(x)$ can be treated as an element of $L^2(-\infty, \infty)$, for which relation (1.4) is valid as pointed out earlier. However, for the same reason, relation (1.4) is valid for the present X and P *only* on the null vector if a is *not* restricted in any way. The function f_m in the calculation above has as its support the entire interval $[0, 2\pi]$, and thus we expect the operator relation (1.4) not to be applicable to it for any $a \neq 0$, a fact which is born out by the calculation above.

Using a formal power series expansion to establish equation (1.4) for a solution to CR (1.1) does not even allow us to conclude as much about the domain of validity of relation (1.4) as is stated in the preceding paragraph. As pointed out in Kraus (1970), for the X and P of our example, CR (1.1) is valid only on the dense set of functions which vanish at 0 and 2π. This comes about because the domain of P is restricted to the periodic functions and

† For a rigorous description of the domain of P see Section 2.11 in Putnam (1967). For a proof of the self-adjointness of P see Section 49 in Akhiezer & Glazman (1961).

because $X\psi$ is periodic only if $\psi(0) = \psi(2\pi) = 0$.† Since expression (1.3) contains terms like $[P, X]P^n$ with arbitrary n, the nth derivative of ψ should vanish at 0 and 2π for arbitrary n so that $P^n\psi$ is in the domain of $[P, X]$. Since $\psi(x)$ should also be analytic in $[0, 2\pi]$ to make the series expansion of $e^{iaP}\psi$, which is used in the formal derivation of equation (1.3) and which is actually just a Taylor expansion around the point x, meaningful, the requirement that all $\psi^{(n)}(0) = 0$ implies that $\psi(x) \equiv 0$ in $[0, 2\pi]$. So the definition of e^{-iaP} in terms of a power series allows us to establish formula (1.4) for the present X and P *only* when it is applied to the null vector. All this goes to illustrate that trying to define an exponential of an unbounded self-adjoint operator in terms of a power series expansion is useful, at best, in special cases only and that manipulating such series formally to derive other operator identities can be expected to lead to results which are either wong or whose domain of validity is difficult to establish from the procedure used in their derivation.

It may be worthwhile to indicate briefly, for the example of the solution of CR (1.1) in $L^2(0, 2\pi)$ considered above, how spectral theory defines exponentials of self-adjoint operators (Jordan, 1969; Yosida, 1971) and how, using this definition, we can evaluate the expectation value $(f_m, e^{iaP}X\, e^{-iaP}f_m)$ considered earlier. If P_m is the projection operator onto the eigenfunction f_m of P belonging to the eigenvalue m, then P can be written

$$P = \sum_m mP_m \tag{1.8}$$

Any vector f in the Hilbert space $L^2(0, 2\pi)$ can be expanded as

$$f = \sum_m (f_m, f)f_m \tag{1.9}$$

Combining equations (1.8) and (1.9), we find the expression used in spectral theory to define Pf,‡

$$Pf = \sum_m m(f_m, f)f_m \tag{1.10}$$

Spectral theory then defines $e^{-iaP}f$ via

$$e^{-iaP}f = \sum_m e^{-iam}(f_m, f)f_m \tag{1.11}$$

† The differentiation operator $-id/dx$ can, of course, also be defined on non-periodic functions; but such an extension of P would make P no longer self-adjoint.

‡ The definition (1.10) of Pf shows that the domain of P is exactly the set of periodic functions because the series on the right converges only for those functions. As an example, consider $f(x) = x$. One look at the Fourier series for $f(x) = x$ will show that the series (1.10) diverges even though $f(x)$ is clearly a well-defined element of $L^2(0, 2\pi)$. This is so because $-id/dx$ is an extension of P which is not self-adjoint; and the example illustrates that the unbounded self-adjoint operator P defined by equation (1.10) should not blindly be replaced by $-id/dx$ and applied to non-periodic functions.

The series (1.11) is convergent for all $f \in L^2(0, 2\pi)$ and all a. Therefore, if

$$Xf_m = \sum_k b_k f_k, \text{ where } b_k = (f_k, Xf_m) \qquad (1.12)$$

we obtain

$$X\, e^{-iaP} f_m = \sum_k e^{-iam} b_k f_k \qquad (1.13)$$

and

$$e^{iaP} X\, e^{-iaP} f_m = \sum_k e^{-iam} b_k\, e^{iak} f_k \qquad (1.14)$$

Therefore the expectation value mentioned above becomes

$$\begin{aligned}(f_m, e^{iaP} X\, e^{-iaP} f_m) &= \sum_k e^{-ia(m-k)} b_k (f_m, f_k) \\ &= b_m \\ &= (f_m, Xf_m) \qquad (1.15)\end{aligned}$$

which agrees with the result in equation (1.6).

Another well-known formula involving exponentials,

$$e^{A+B} = e^A e^B e^{-1/2[A,B]}, \qquad \text{where } [A, [A,B]] = [B, [A,B]] = 0 \qquad (1.16)$$

also is not valid for the operator pair X, P in $L^2[0, 2\pi]$ considered above. As formula (4.1), formula (1.16) is derived by formal power series expansion or equivalent procedures. This formula, also, is often quoted either with the explicit comment that it is valid for *any* two operators A and B which commute with their commutator (Glauber, 1951; Gottfried, 1966) or, at least, without any other comment about restrictions on its validity (Messiah, 1966).

Let us close now by considering Weyl's CR(2). It is a special case of formula (1.16). To see this, set $A = iaP, B = ibX$, and evaluate $e^{iaP}e^{ibX}$ and $e^{ibX}e^{iaP}$ using formula (1.16) and CR (1.1). To see explicitly that CR (1.2) is invalid for the operator pair X, P in $L^2(0, 2\pi)$ considered above, calculate the expectation value for the two sides of CR (1.2) for the eigenstate f_m of P. The two expectation values are not equal.

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