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The Importance of the Domain of Operators in Quantum Mechanics

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Abstract This paper aims to examine the significance of the domain of operators in the mathematical and physical structure of quantum mechanics. Specifically, we explore the distinction between observable self-adjoint and Hermitian operators, determined by their respective domains. We also discuss the Algebra of unbounded operators with the concept of the domain of operators. Our analysis reveals that creation and annihilation operators are not generally self-adjoint towards each other in standard quantum mechanics, as demonstrated through mathematical equations.

1 Introduction

Quantum mechanics is based on the algebra of the linear operators, which are responsible for observables in the quantum world [1]. The distinction between Hermitian and self-adjoint operators is contingent upon the domain of operators, which has a vital contribution in this context. Additionally, integrable functions exhibit quadratic behaviour and do not vanish at infinity. Notably, despite this characteristic, the momentum operator does not conform to Hermiticity criteria. However, it is essential to recognize that these functions are separate from the domain of the momentum operator (as their differentiations are often non-square-integrable). Mathematicians consider every operator in Hilbert space to have two essential properties. The first is the action of an operator, and the second is its domain. The action of an operator refers to its effect on the functions it is applied to, such as differentiation or integration. An operator's domain is a specific set of functions that the operator acts on. While quantum mechanics literature often neglects to mention the domain of operators, the importance of an operator domain is highlighted in distinguishing between self-adjoint and Hermitian operators [2]. We start the discussion with the definition of the adjoint operator, which can be seen in quantum mechanics literature. However, recently, it has been reported that this subject is adjoint to an operator beyond the textbooks [3].

Definition: Assume that a densely defined operator A with domain $D(A)$, and its adjoint A^* with domain $D(A^*)$. According to the definition, the following relationship holds for all functions f and g:

$$(A*f,g)=(f,Ag). \tag{1}$$

We use a symbol like that employed in math literature for reasons that will become clear later.

Now, the following two definitions can be mentioned:

1. An (densely defined) operator A is Hermitian (or symmetric in mathematics literature) provided that its action is the same as the action of A* and $D(A)\subseteq D(A*)$. The condition $D(A)\subseteq D(A*)$follows from the definition of A^*.
2. An (densely defined) operator A is self-adjoint, again, provided that its action is the same as that of A*. But, in this case

$$D(A)=D(A*),$$

According to this definition, all bounded operators are self-adjoint.

Note that the domain of A is obtained from Eq. (1).

2 Position operator

The position operator in quantum mechanics is an unbounded operator, which is never defined on the entire Hilbert Space and inevitably, the domain related to such must be considered. This operator on the real axis is defined as follows [4]:

$$X\Psi(x)=x\Psi(x),\ x\in\mathbb{R},\Psi(x)\in L^2(\mathbb{R},dx), \tag{2}$$

and the domain of the position operator is equal to:

$$D(X)=\{\Psi(x)\in L^2(\mathbb{R},dx)\mid\int x^2\,|\Psi(x)|^2\mathrm{dx}<\infty\}. \tag{3}$$

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The following lemma can be deduced from the action type and the position operator's definition.

Lemma 1 *If the measurement on the position of a particle leads to an upper limit, which means:* $\lim_{x\to\infty}|x\Psi(x)| = 0.$ *So, the desired continuous state function must be square integrable.*

Proof We separate the integration domain into following three parts: $[-1,1]$, $(-\infty,-1]$, $[1,+\infty)$.

For the first interval, since $\Psi(x)$ is continuous, then $|\Psi(x)|^2$ is also continuous. Therefore, $\int_{-1}^{1}|\Psi(x)|^2\, dx$ is finite. Now we examine the interval $[1,+\infty)$. From the postulation of the lemma, we conclude that there is a positive constant such as k, which can be written for all $x \geq 1$, as $|x\Psi(x)|\langle k$, so we have:

$$\int_1^\infty |\Psi(x)|^2 dx < \int_1^\infty \frac{k^2}{x^2} dx = k^2.$$

A similar argument holds for the interval $(-\infty,-1]$.

3 Momentum operator

The momentum operator is an unbounded operator whose domain is as follows [4].

$$D(P) = \{\Psi(x) \in L^2(\mathbb{R}, dx) | \Psi'(x) \in L^2(\mathbb{R}, dx)\}. \quad (4)$$

It is noteworthy, concerning the domain of momentum operator, there are square-integrable functions that its derivatives do not exist in $L^2(\mathbb{R}, dx)$. Hence, they do not belong in the domain of the momentum operator. For example, consider a function $f(x) = \frac{x^{\frac{1}{3}}}{1+x^2}$, despite this fact that it is considered to be a square-integrable function, but its derivative is not. Therefore, this function does not satisfy the requirement for inclusion in the domain of the momentum operator. In general, for $f(x)$ and $g(x)$ which belong to the domain of momentum operator one can write:

$$(g, Pf) - (Pg, f) = (-i\overline{g}f)_{-\infty}^{+\infty},$$

where f and g functions are often considered to be equal to zero when $x \to \pm\infty$.

It is important to note that not all square-integrable functions lead to zero, as they tend to infinity [5].

For instance, consider the function $f(x) = \sqrt{\cos x^2}$ which is square-integrable, but does not vanish when the amount of X tends to infinity. However, this is not of concern to us. In this case, see the following lemma:

Lemma 2 *Every square-integrable function that belongs to the domain of momentum operator will certainly vanish as they tend towards infinity (given their continuity and smoothness).*

Proof Consider g to be the conjugated form of function f, which is also square-integrable. Since $f \in D(P)$, then $f' \in L^2(\mathbb{R})$, and the inner product of (g, f') is well defined, we can also write:

$$(g, f') = \frac{1}{2}\int_{-\infty}^{+\infty}(f^2)'dx = f^2(+\infty) - f^2(-\infty).$$

It is clear that the limit of f^2 exists as it tends to infinity. It follows that both f^2 and $|f|^2$ tend to finite limits as infinity is approached. If any of the mentioned limits were equal to a number other than zero, the integral of $|f|^2$ would tend to infinity over the domain of real numbers, which contradicts the square-integrability of the f function. Consequently, both $|f|^2$ and f tend to zero when $x \to \pm\infty$.

A similar discussion but for generalized momentum operators can be found in [6].

4 Algebra of unbounded operators

The main distinction between bounded and unbounded operators lies in their domains [4]. The domain of an unbounded operator is a suitable subspace of Hilbert Space, thereby rendering certain algebraic operations such as addition and multiplication distinct from those about bounded operators. To illustrate the latter, consider two unbounded operators, A and B, and assume their sum to be $a = A + B$. According to Eq. (1) and for $f, g \in D(a)$ one can write:

$$(g, af) = (g, (A+B)f) = ((A+B)^*g, f). \quad (5)$$

By rewriting the Eq. (5), we conclude that:

$$((A^* + B^*)g, f) = ((A+B)^*g, f). \quad (6)$$

In this equation that A and B are unbounded, it is possible that $(A^* + B^*)g$ may not exist. However, if A and B are bounded, their domains coincide with Hilbert Space, thereby, obviating such concerns.

Theorem 1 *Consider two operators A and B, therefore:*

$$D(A+B)^* \supset D(A^* + B^*). \quad (7)$$

An interesting and impressive example for Eq. (7) is considering $A = -B$, it is obvious that $D(A) = D(B)$ and $D(A^*) = D(B^*)$. Now we assume that the domain of operator A is not the whole of Hilbert Space, while the domain of the operator B is whole of Hilbert space. So

$$D(A^* + B^*) = D(A^*) \cap D(B^*) = D(A^*).$$

Moreover, it follows that $D(A+B)^* = 0$, encompasses all of Hilbert Space. It is an exact confirmation of Theorem 1.

Wherein the Hermitian part of an arbitrary operator A may be obtained as below:

$$A^H = \frac{A+A^*}{2}. \tag{8}$$

Now, concerning our discussion in this section, one can write:

$$D(A+A^*)^* \supset D(A^*+A^{**}).$$

Thereby:

$$D(A^H)^* \supset D(A^H). \tag{9}$$

This conclusion again confirms the definition of Hermitian operator (according to the condition $A^{**} = A$).

As previously discussed, a requisite condition for Eq. (7) validity is associated with the boundedness of at least one of the involved operators. However, this criterion does not hold for the position and momentum operators, which are both unbounded. These two operators are exceptions in that Eq. (7) holds for them despite their unbounded nature.

Theorem 2 *Assume the inner product of densely defined A and B operators, then* $(BA)^* \supset A^*B^*$.

For both Theorems, equality is assured by the boundness of one of the operators A or B [7, 8]. In contrast, for Theorem 2, equality would be obtained by another condition that one of the operators should be invertible, and the inverse operator must be bounded [7]. The equality of Theorem 2 can be proved without considering the domain of operators. (Even though paying attention to the domain of operators is considered to prove the equality of this Theorem.)

Assume that, A is an invertible operator.

$$AA^{-1} = I. \tag{10}$$

By multiplying B in both sides we have:

$$BAA^{-1} = B,$$

and by supposing that A^{-1} is bounded one can write:

$$(A^{-1})^*(BA)^* = B^*. \tag{11}$$

According to the fact that $(A^{-1})^* = (A^*)^{-1}$, we conclude:

$$(BA)^* = A^*B^*. \tag{12}$$

Despite what has been mentioned in the latter, none of the mentioned states apply to the equality states of position or momentum operators. Since the mentioned operators are unbounded, the momentum operator is invertible, not bounded. The inverse momentum operator and its domain are:

$$\frac{1}{P} = i\int_{-\infty}^{x} dx\, D\left(\frac{1}{P}\right)$$
$$= \{\Psi(x) \in L^2(\mathbb{R}, dx) | \int_{-\infty}^{+\infty} \Psi(x')\, dx' = 0.$$

This operator and its generalization in the curved space have been reported in [9].

Now, pay attention to the sum of the two operators. If unbounded operators A and B are Hermitian so the sum of them is also Hermitian. Note that, if both operators were self-adjoint, it would not be obtained that their sum is also self-adjoint [4]. Therefore, considering $A \subset A^*$, and $B \subset B^*$ one can write:

$$(A+B)^* = (A+B) \subset A^* + B^*. \tag{13}$$

Regarding $(A+B)^* \supset A^* + B^*$, (Theorem 1), it is clear that

$$(A+B)^* = A^* + B^*. \tag{14}$$

5 The relationship between creation and annihilation operators

In quantum mechanics, literature, creation and annihilation operators are introduced as complex linear combinations of position and momentum operators, which consist of $a = X + iP$ and $a^\dagger = X - iP$ [1]. These operators are defined with constant coefficients assumed to be one (It should be noted that $*$ symbol is used for an adjoint operator).
For $f \in D(a)$ and $g \in D(a^*)$ we can write:

$$(g, (X+iP)f) = ((X+iP)^*g, f).$$

The left-hand side of the equation will be equal to:

$$(g, Xf) + (g, iPf) = \big((X-iP)g, f\big).$$

In this way, every function g that is in the domain of $a^\dagger$ must also be in the domain of a^*, so it can be concluded:

$$a^\dagger \subset a^*. \tag{15}$$

Similarly, it can be obtained that:

$$a \subset (a^\dagger)^*. \tag{16}$$

It can be concluded that the operators a and $a^\dagger$ are merely a definition and are not generally adjoint to each other.

6 Conclusion

This paper emphasises the crucial role played by the domain of operators in distinguishing between self-adjoint and Hermitian operators. Furthermore, we note that the momentum operator is not self-adjoint due to the existence of certain square-integrable functions that do not vanish at infinity; however, these functions do not belong in the domain of the momentum operator. Finally, we present our findings on the relationship between creation and annihilation operators in quantum mechanics, which are introduced as being adjoint of each other but have shown not to be generally adjoint of each other.

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