Some impressive properties of unbounded operators in quantum mechanics

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Abstract

In this paper we have presented the necessity of defining the domain of the operators in quantum mechanics. We have investigated some controversial issues concerning algebra of unbounded operators. Our main focus has been the position and momentum operators. We have also shown the necessity of the presence Schwartz functions in quantum mechanics. The original aim of this paper is to present some mathematical issues of quantum mechanics in an understandable form for physics students.

Keywords: Unbounded operator- bounded operator- Schwartz space.

Resumen

En este artículo hemos presentado la necesidad de definir el dominio de los operadores en mecánica cuántica. Hemos investigado algunas cuestiones controvertidas relativas al álgebra de operadores ilimitados. Nuestro principal enfoque ha sido los operadores de posición e impulso. También hemos demostrado la necesidad de la presencia de funciones de Schwartz en la mecánica cuántica. El objetivo original de este artículo es presentar algunas cuestiones matemáticas de la mecánica cuántica de una forma comprensible para los estudiantes de física.

Palabras clave: Operador ilimitado- operador acotado- Espacio de Schwartz.

I. INTRODUCTION

There is a well-known reference concerning advanced mathematical subjects in physics. For example, algebra operators in quantum mechanics [1]. However, this book is not relatively simple for students. In this regard, some people have tried to understand some of the mathematical concepts of quantum mechanics for students [2, 3, 4]. Here we intend to express some modern mathematical concepts in understandable forms. At first, we introduce the domain of the operators and indicate that they have an important contribution in distinction between self-adjoint and Hermitian operators. Furthermore, we introduce bounded and unbounded operators in a nutshell. Then after mentioning some of the operator's algebraic properties, we introduce Schwartz space and functions. Finally, we investigate the discontinuity of the wave functions by considering that they are into the domain of the position and momentum operators or not.

II. DOMAIN OF AN OPERATOR

From a mathematical point of view, every operator in the Hilbert space has two important points: the operator's action and its domain [2]. The action is what the operator does to the functions on which it acts. The domain is the specified set of functions on which the operator acts [2]. Basically, quantum mechanics text books do not refer to the domain of the operators [2, 4]. Of course, there are many mathematical points which are not extensively discussed in text books of quantum mechanics. Perhaps there is not enough space or background to discuss them.

An operator A , on the Hilbert space H is a linear map

$$A: D(A) \rightarrow H,$$
$$\psi \rightarrow A\psi,$$

where $D(A)$ represents a dense linear subspace of H. This subspace is called the domain of A [5].

The necessity of definition of the domain in quantum mechanics is determined when we encounter the functions which are square-integrable but does not vanish at infinity. Some examples of such functions are available (Mathematical Surprises and Dirac's Formalism in Quantum Mechanics, F. Gieres, 2001) [5]. Later on, we will investigate this issue in other part.

An operator A on a Hilbert space H is said to be Hermitian (or symmetric in mathematics literatures), if we have

$$\langle g, Af\rangle = \langle Ag, f\rangle \text{ for all } g, f \in D(A) \text{ and}$$
$$D(A) \subset D(A^*) .$$

An operator A on a Hilbert space H is said to be Self-adjoint, if A is densely defined and $D(A) = D(A^*)$.

Indeed, why is the domain of the adjoint of the operator bigger than the domain of the operator itself for Hermitian operators? Is there a proof for that or it is only a definition?

Suppose the domain of A^* is the set of all members x in the Hilbert space such as g_x with

$g_x(y) = \langle x, Ay \rangle$ is well-defined and continuous on the domain of A. Now consider z in the domain of A. For all $y \in D(A)$ we can write $g_z(y) = \langle z, Ay \rangle = \langle Az, y \rangle$ as A is Hermitian. Also, the right- hand side is continuous in terms of y, as it is the inner product of something with y. So g_z is well-defined and continuous on $D(A)$, which means that z is in the domain of A^*. That is any member of the domain of A is a member of the domain of A^*. Hence A is a subset of A^*.

Note that in this paper we use * symbol for the adjoint of operators, similar to mathematics literature.

III. BOUNDED OPERATORS

A linear operator $A: H \rightarrow H$ is bounded if and only if there is a constant c such that for all vectors $\psi \in D(A)$, we have

$$||A|| \leq c||\psi||, \tag{1}$$

where we mean by$||A||$ the norm of A. Clearly the above condition indicates that the spectrum of A is bounded [1]. Some of the important examples of bounded operators in quantum mechanics are unitary operators, projection operators and parity.

IV. UNBOUNDED OPERATORS

The truth is that in most cases, we deal with unbounded operators in quantum mechanics. On the other hand, from a philosophical perspective [6] employing of unbounded operators in quantum mechanics leads directly to a kind of incompleteness.

For these operators the condition (1) does not always hold. In fact, they are never defined on the whole Hilbert space and we have to consider the respective domain of these operators.

The most important unbounded operators in quantum mechanics are position and momentum. The position operator X for a particle on the real line is the multiplication by x on $L^2(\boldsymbol{R}, dx)$

$$X\psi(x) = x\psi(x), \qquad \text{for all } x \in \boldsymbol{R}.$$

The maximal domain of position operator is the one which ensures that the function $X\psi$ exists and it still belongs to the Hilbert space

$$D_{max}(X) = \{\psi \in H\} = \left\{\psi \in L^2(\boldsymbol{R}, dx)|, \quad ||X\psi||^2 \equiv \int dx\, x^2 |\psi(x)|^2 < \infty\right\}. \tag{2}$$

From the action of the position operator and its domain we simply conclude it is essential that $\lim_{x \to \pm\infty} |x\psi(x)| = 0$.

The maximal domain of the momentum operator $P = -i\frac{\partial}{\partial x}$ also on the Hilbert space $L^2(\boldsymbol{R}, dx)$ is

$$D_{max}(P) = \{\psi \in H\} = \begin{Bmatrix} \psi \in L^2(\boldsymbol{R}, dx)| \\ \psi' \in L^2(\boldsymbol{R}, dx) \end{Bmatrix}. \tag{3}$$

In the definition of (3), $\psi' \in L^2(\boldsymbol{R}, dx)$ means that the derivative ψ' exists almost everywhere and belongs to $L^2(\boldsymbol{R}, dx)$ [5]. For example, consider a following square-integrable function

$$f(x) = \frac{x^{\frac{1}{3}}}{1+x^2}.$$

One easily finds that the derivative of $f(x)$ is not square-integrable and then does not belong to the momentum operator.

According to the definition of momentum operator and using integration by parts one can get

$$(g, Pf) - (Pg, f) = [-i\overline{g(x)}f(x)]_{-\infty}^{\infty}. \tag{4}$$

Since f and g are square integrable, one usually concludes that these functions vanish for $x \rightarrow \pm\infty$ [5]. However, as mentioned in section II, not all square-integrable functions vanish at infinity or even to a finite value. There are plenty counterexamples for that. However, most of these functions do not satisfy the condition (3). Now a delicate question can be pointed out. Is there any function with this property, which is square-integrable but it doesn't tend to zero at infinity, but to be in the domain of the momentum operator? The short answer is: No. There is no such function.

One can find the exact solution to this question in [7]. Note that in ref. [7] is used from modern mathematical concept such as "weak derivative" but here we provide a simpler argument. Also, there is a similar discussion concerning generalized momentum operators in research done by M. Jafari Matehkolaee, 2021 [8]. As for the research for the momentum operators in curved spaces (M. Jafari Matehkolaee, 2019 and 2023 respectively) [9, 10] and their references, suppose f is such a function which mentioned in above question. Let's call it complex conjugate, that is $\bar{f} = g$. As f is square-integrable so is g. Also, we assume that f is member of the momentum operator hence according to (3), f' is also square-integrable. This indicates that (g, f') is well-defined. One can write

$$(g, f') = \frac{1}{2}\int_{-\infty}^{+\infty} (f')^2 dx. \tag{5}$$

This integral is equal to the limit of $R \rightarrow +\infty$ and $S \rightarrow -\infty$ of $[f^2(R) - f^2(S)]$. Clearly this limit exists means that the limit of $f^2(R)$ as $R \rightarrow +\infty$ exists and the limit of $f^2(S)$ as $S \rightarrow -\infty$ exists. In general, we cannot infer that both limits exist; only their difference exists. But in our case, it is true. So f^2 tends to some limits for $+\infty$ and $-\infty$. Hence $|f|^2$

tends to some limits for $+\infty$ and $-\infty$. If either of those limits is nonzero, then the integral of $|f|^2$ over the real line will be infinite. But as f is square-integrable this cannot happen. So $|f|^2$ tends to zero at both plus and minus infinity, and hence f tends to zero at these limits.

V. ALGEBRAIC PROPERTIES OF OPERATORS

It is seen, the basic difference between bounded operators and unbounded operators is the domain on which they are defined. Domains of unbounded operators are proper subspaces of Hilbert space. Because of this fact, many aspects of the theory of unbounded operators are somewhat counterintuitive. For example, the algebraic rules for sums and products break down.

Theorem:

1) Let A and B be operators so that $(A+B)$ is densely defined then $(A+B)^* \supset A^*+B^*$.

The proof of this theorem is in [11]. However, let us provide a simple example. Consider $B=-A$ then, obviously the domains of A and B are the same and the case is the same for A^* and B^* as well. But it could happen that the domain of A^* is not the whole Hilbert space then the domain of A^*+B^* is the same as the domain of A^*, while $A+B=0$ so that the domain of $(A+B)^*$ is the whole Hilbert space.

Now we can provide another instance. As we know the Hermitian part of arbitrary operator is given by

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

According to the above theorem one can write

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

If we assume that $A^{**}=A$, then one can conclude

$$D(A^H)^* \supset D(A^H).$$

This conclusion is completely consistent to the definition of the Hermitian operators in section II.

The proof of this theorem can also be seen in research by J. Weidmann (1980) and Akhiezer-Glazman (1981) respectively [11, 12].

The equality situation is guaranteed if one of the operators is bounded [11, 12]. But in the latter case, if one of the operators is bounded inversely, then the equality is persuaded [11]. For example, A is invertible and A^{-1} is bounded, then we can show that $(BA)^* = A^*B^*$. In this case, we can argue without using of the domain of the operators (it will be different from what was expected by J. Weidmann's research [11]) so consider

$AA^{-1}=I$ then $BAA^{-1}=B$ and one can write $(BAA^{-1})^*=B^*$ since A^{-1} is assumed to be bounded so it's safe to write $(A^{-1})^*(BA)^*=B^*$ and hence

$$(BA)^* = A^*B^*.$$

Unfortunately, none of these conditions is valid for position and momentum operators. The operators X and P are unbounded and although P is invertible, the momentum inverse operator $\frac{1}{P}$ is not bounded.

$$\frac{1}{P} = i\int_{-\infty}^{x} dx',$$
$$D\left(\frac{1}{P}\right) = \left\{\psi(x) \in L^2(\boldsymbol{R}, dx) \mid \int_{-\infty}^{\infty}\psi(x')dx' = 0\right\}. \quad (6)$$

How can the equality of the theorem be concluded? In particular to deal with the operators X and P, i.e., how is the relationship between $(X+P)$ and its adjoint?

Now at first, consider $a=A+B$. According to the definition of the adjoint of the operator one can write, $f, g \in D(a)$,

$$(g, af) = (g,(A+B)f) = ((A+B)^*g, f), \quad (7)$$

or

$$(g, af) = (g,(A+B)f) = (g, Af) + (g, Bf) = ((A^*+B^*)g, f). \quad (8)$$

It seems that we can conclude that

$$((A+B)^*g, f) = \big((A^*+B^*)g, f\big). \quad (9)$$

However, the vector $(A^*+B^*)g$ might not even exist since the operators A and B are unbounded. We know, in general, what the theorem (1) says is true. However, if the domains are equal then it is not a problem and this is exactly the difference between bounded and unbounded operators since in the bounded case the domain of the operator is the whole Hilbert space and we do not have to specify its domain.

Fortunately, there is a space called Schwartz space in which represents an invariant domain for the position and momentum operators [5]. Therefore, the concern we had about Hilbert space's functions at infinity now we do not have in Schwartz space.

VI. THE NECESSITY OF SCHWARTZ FUNCTIONS IN QUANTUM MECHANICS

There is a delicate point in Quantum Physics (S. Gasiorowicz, 2003) [13] concerning square-integrable functions:

"Since we may need to deal with integrals of the type

$$\int_{-\infty}^{\infty} \overline{\psi(x,t)}\, x^n\, \overline{\psi(x,t)} dx, \quad (10)$$

and

$$\int_{-\infty}^{\infty} \overline{\psi(x,t)}\, \left(\frac{\partial}{\partial x}\right)^n \overline{\psi(x,t)} dx. \quad (11)$$

We will require that the wave functions $\psi(x,0)$ go to zero rapidly as $x \to \pm\infty$, often faster than any power of x ".

From this statement, we find that wave functions must have certain characteristics. For example, they should be continuous, differentiable and bounded at infinity. As we have seen, all of the square-integrable functions in Hilbert space do not have these properties.

Instead, in Schwartz space, functions are smooth, i.e., one can differentiate those infinite times. Also, Schwartz functions are called functions of rapid descent. That is along with their derivatives, as $|x| \to \infty$ they tend to zero faster than any inverse power of x does.

The space of all Schwartz functions is called Schwartz space, and it is denoted by $S(\boldsymbol{R}^n)$.

the Schwartz space $S(\boldsymbol{R})$ is the vector space of smooth functions $f: R \to \mathbb{C}$, such that for all $n, m = 0,1,2, \ldots$, we have

$$\lim_{x \to \pm\infty} \left| x^n \frac{d^m f}{dx^m} \right| = 0. \quad (12)$$

It can be shown that $X\psi(x) = x\psi(x)$ defines a map $X: S(\boldsymbol{R}) \to S(\boldsymbol{R})$, also $Pf = -i\frac{\partial}{\partial x}f$ defines a map $P: S(\boldsymbol{R}) \to S(\boldsymbol{R})$. It is easily seen that position and momentum operators have a common domain of self-adjointness in Schwartz space. Since X and P in Schwartz space are symmetric so one can write $(X + P) \subset X^* + P^*$ or $(X + P)^* \subset X^* + P^*$ and according to theorem (1) one can conclude that $(X + P)^* = X^* + P^*$.

There are two operators in quantum mechanics which are introduced as creation and annihilation operators so that those are linear complex combination of position and momentum operators. These operators are given by

$$a = (X + iP) \text{ and } a^+ = (X - iP).$$

where we assumed constant coefficient equals one. In textbooks of quantum mechanics a and a^+ are considered the adjoint of each other, but actually they are not the adjoint one of the other [14]. Here we can indicate a^+ can be just a restriction of the adjoint of a to a suitable domain.

For $f \in D(a)$ and $g \in D(a^*)$ we can write:

$$(g, (X + iP)f) = ((X + iP)^* g, f). \quad (13)$$

The left-hand side is equals to:

$$(g, Xf) + (g, iPf) = \Big(\big((X - iP) \big) g, f \Big). \quad (14)$$

One can conclude $\in D(a^+)$, that every g which is member of the domain of a^+ is a member of the domain of a^* hence

$a^+ \subset a^*$ and it can be shown similarly $a \subset (a^+)^*$.

It seems we should stress that if one deals with Schwartz space, the momentum operator one find is not self-adjoint but it is only Hermitian. That non-self-adjoint operator is however essentially self-adjoint which means that it admits a unique self-adjoint extension. This unique extension is the true momentum operator of quantum mechanics. Indeed, usually one uses Schwartz space for two reasons. (1) The true momentum operator is uniquely determined by its restriction to Schwartz space. (2) In the Schwartz space, the said restriction is nothing but a standard derivative $-i\frac{\partial}{\partial x}$, so there the momentum operator is a differential operator. The true momentum operator is not a differential operator because the notion of derivative one uses is the weak derivative [14].

VII. CONCLUSION

We have reviewed some of the properties bounded and unbounded operators and their algebraic properties. We have indicated that Schwartz functions are necessary to justify some unbounded operator's algebraic relationships. Herein, we have investigated the discontinuity of the functions which are square-integrable and member of the position operator. However, we can mention examples which are square-integrable, but not in the domain of the position operator nor momentum operator, an example can be found in Unbounded Operators and the Incompleteness of Quantum Mechanics (A. Heathcote, 1990) [6]. For these functions also one can use the same way we mentioned here.

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