On the connection between the Schrödinger and the Heisenberg pictures for unbounded operators

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Abstract. It is well known that the unboundedness of operators in Hilbert space entails domain troubles. It is also well known that most domain troubles can be surmounted by extending the Hilbert space to a rigged Hilbert space. In this note, we point out another of such troubles, namely the correspondence between the Schrödinger and the Heisenberg pictures for unbounded operators, and sketch the solution of this problem within the rigged Hilbert space.

1. Introduction

Quantum Mechanics textbooks show that the Schrödinger and the Heisenberg pictures are physically equivalent, because they yield the same probability amplitudes for measuring an observable A in a state φ. Textbooks, however, usually omit the fact that for unbounded operators, the manipulations that lead from the Schrödinger to the Heisenberg picture must be taken with care, due to domain problems. The purpose of this note is to point out those domain problems and to sketch their solution by extending the Hilbert space to the rigged Hilbert space. For a class of potentials, we use a theorem by Hunziker to solve such problems explicitly.

2. The problem

Suppose that the algebra $\mathscr{A}$ of observables of a system consists of the following operators:

$$\mathscr{A} = \{H, A_1, A_2, \ldots, A_N\}\,, \tag{1}$$

where H is the Hamiltonian and $A_1, A_2, \ldots, A_N$ are the other relevant observables of the system (e.g., position and momentum). Those operators are assumed to be self-adjoint on a Hilbert space $\mathscr{H}$. For simplicity, we restrict ourselves to pure states and to observables that do not depend explicitly on time. Then, in the Schrödinger picture, which shall be denoted by the subscript S, the observables are kept fixed in time,

$$A_{\mathrm{S}}(t) = A_{\mathrm{S}}(0) = A\,, \tag{2}$$

whereas the states evolve in time according to the Schrödinger equation,

$$i\hbar\frac{d}{dt}\varphi_{S}(t)=H\varphi_{S}(t)\,. \tag{3}$$

Integration of this equation leads to

$$\varphi_{S}(t)=e^{-iHt/\hbar}\varphi_{S}(0)\equiv e^{-iHt/\hbar}\varphi\,. \tag{4}$$

In the Schrödinger picture, the expectation value of the measurement of the observable A in the state φ is given by

$$\langle A\rangle_{S}(t)=\langle\varphi_{S}(t)|A_{S}|\varphi_{S}(t)\rangle=\langle e^{-iHt/\hbar}\varphi|A|e^{-iHt/\hbar}\varphi\rangle\,. \tag{5}$$

In the Heisenberg picture, which shall be denoted by the subscript H, the states are kept fixed in time,

$$\varphi_{H}(t)=\varphi_{H}(0)=\varphi\,, \tag{6}$$

whereas the observables evolve in time according to "Heisenberg's equation of motion:"

$$i\hbar\frac{d}{dt}A_{H}(t)=[A_{H}(t),H]\,. \tag{7}$$

In integrated form, Eq. (7) reads as

$$A_{H}(t)=e^{iHt/\hbar}A_{H}(0)e^{-iHt/\hbar}=e^{iHt/\hbar}Ae^{-iHt/\hbar}\,. \tag{8}$$

In the Heisenberg picture, the expectation value of the measurement of A in the state φ is given by

$$\langle A\rangle_{H}(t)=\langle\varphi_{H}|A_{H}(t)|\varphi_{H}\rangle=\langle\varphi|e^{iHt/\hbar}Ae^{-iHt/\hbar}|\varphi\rangle\,. \tag{9}$$

The equivalence of the Schrödinger and Heisenberg pictures is guaranteed by the equality of the expectation values (5) and (9):

$$\langle A\rangle_{S}(t)=\langle A\rangle_{H}(t)\,, \tag{10}$$

which follows from the unitarity of the group evolution operator $e^{-iHt/\hbar}$.

When the operators of the algebra $\mathscr{A}$ are all bounded, they are defined on the whole of the Hilbert space $\mathscr{H}$, and domain troubles do not arise. But if at least one operator of the algebra, say A_1, is unbounded, then A_1 cannot be defined on the whole of the Hilbert space, but at the most on a dense subspace $\mathscr{D}(A_1)$ of the Hilbert space on which A_1 is self-adjoint. In such event, one has to specify on what states the algebraic operations involving unbounded operators are valid, since algebraic operations (e.g., sums, products and commutation relations) of unbounded operators are not defined on the whole of $\mathscr{H}$: If A and B are two unbounded operators defined on two dense subdomains $\mathscr{D}(A)$ and $\mathscr{D}(B)$ of $\mathscr{H}$, then the sum of A and B, $A+B$, is defined only for $f\in\mathscr{D}(A)\cap\mathscr{D}(B)$; the product of A by B, BA, is defined only for those $f\in\mathscr{D}(A)$ such that $Af\in\mathscr{D}(B)$; the commutation relation of A and B, $[A,B]=AB-BA$, is defined only for those f such that $f\in\mathscr{D}(A)\cap\mathscr{D}(B)$, $Af\in\mathscr{D}(B)$ and $Bf\in\mathscr{D}(A)$.

Likewise algebraic operations, the time evolution (8) of an unbounded operator A cannot be defined on the whole of $\mathscr{H}$. Clearly, the time evolution of A,

$$A(t)\equiv e^{iHt/\hbar}Ae^{-iHt/\hbar}\,, \tag{11}$$

is defined only for those $f\in\mathscr{H}$ such that $e^{-iHt/\hbar}f\in\mathscr{D}(A)$. Thus, the Heisenberg picture of an unbounded operator A is not defined on the whole of $\mathscr{H}$.

We have therefore to face the fact that algebraic operations and the Heisenberg picture of unbounded operators entail domain troubles. As we are going to see in the next section, such domain troubles can be surmounted by extending the Hilbert space to the rigged Hilbert space.

3. Sketch of a solution

The way the rigged Hilbert space surmounts the domain troubles of algebraic operations is well known (see [1] for a recent, simple example). Basically, when resonances are not involved, one has to construct the maximal invariant subspace of the algebra of operators,

$$\Phi = \bigcap_{A\in\mathscr{A}} \mathscr{D}(A) \, . \tag{12}$$

The space Φ is obviously contained in the domains of the observables of the algebra,

$$\Phi \subset \mathscr{D}(A) \, , \quad A \in \mathscr{A} \, , \tag{13}$$

and is the largest subspace of the Hilbert space that remains invariant under the action of all the operators of the algebra:

$$A\Phi \subset \Phi \, , \qquad A \in \mathscr{A} \, . \tag{14}$$

It is precisely this invariance what makes all algebraic operations (e.g., sums, multiplications and commutation relations) well defined on Φ. In addition, the bras $\langle a|$ and the kets $|a\rangle$ associated with the continuous spectra of the operators belong to the dual, Φ', and to the antidual, $\Phi^\times$, spaces, respectively:

$$\begin{aligned} &\langle a| \in \Phi' \, , \\ &|a\rangle \in \Phi^\times \, . \end{aligned} \tag{15}$$

Now, it is clear that in order to avoid the domain troubles of the time evolution (11) of an unbounded observable A, we simply need to let $A(t)$ act on a subspace whose time evolution is included in $\mathscr{D}(A)$. Since we want this to happen for all the operators of the algebra, it is natural to demand that the space Φ be invariant under the action of the time evolution group:

$$\mathrm{e}^{-\mathrm{i}Ht/\hbar}\Phi \subset \Phi \, . \tag{16}$$

When the invariance (16) holds, the time evolution of all the operators of the algebra is well defined on Φ, and Φ is invariant under $A(t)$:

$$A(t)\Phi \subset \Phi \, , \qquad A \in \mathscr{A} \, . \tag{17}$$

This invariance makes, in particular, all algebraic operations involving the time evolution of the observables well defined.

The problem is, it is not known whether the invariance (16) holds for any Hamiltonian and for any algebra we could think of. But, as we are going to see in the next section, for some cases of interest a theorem by Hunziker provides a positive answer.

To finish this section we note that, as a byproduct of the invariance (16), one can define the time evolution of the bras and kets:

$$\begin{aligned} &\langle a|(t) = \langle a|\mathrm{e}^{\mathrm{i}Ht/\hbar} \, , \\ &|a\rangle(t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}|a\rangle \, . \end{aligned} \tag{18}$$

In the rigged Hilbert space language, the precise definition of this time evolution is as follows:

$$\begin{aligned} &\langle a|\mathrm{e}^{\mathrm{i}Ht/\hbar}|\varphi\rangle \equiv \langle a|\mathrm{e}^{-\mathrm{i}Ht/\hbar}\varphi\rangle \, , \quad \varphi \in \Phi \, , \\ &\langle \varphi|\mathrm{e}^{-\mathrm{i}Ht/\hbar}|a\rangle \equiv \langle \mathrm{e}^{\mathrm{i}Ht/\hbar}\varphi|a\rangle \, , \quad \varphi \in \Phi \, . \end{aligned} \tag{19}$$

Because $\langle a|$ and $|a\rangle$ are defined only when they act on Φ, definitions (19) make sense only when $\mathrm{e}^{-\mathrm{i}Ht/\hbar}\varphi$ and $\mathrm{e}^{\mathrm{i}Ht/\hbar}\varphi$ belong to Φ; that is, definitions (19) make sense only when Φ is invariant under the time evolution group. Thus, the invariance of Φ under the time evolution group, which guarantees that $A(t)$ is well defined, also guarantees that the time evolution of the bras and kets is well defined.

4. Example

In practical applications, the most important unbounded observables we encounter are the position, the momentum and the energy operators. If, for simplicity, we restrict ourselves to one dimension, the position operator Q is defined as multiplication by the position coordinate:

$$Qf(x) = xf(x)\,; \tag{20}$$

the momentum operator P is defined as differentiation with respect to the position coordinate:

$$Pf(x) = -\mathrm{i}\hbar\frac{\mathrm{d}f(x)}{\mathrm{d}x}\,; \tag{21}$$

and the energy operator, or Hamiltonian, H is the sum of the kinetic energy operator and the potential $V(x)$:

$$Hf(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 f(x)}{\mathrm{d}^2 x} + V(x)f(x)\,. \tag{22}$$

As we explained in the previous section, we have to construct the maximal invariant subspace Φ of the algebra $\{H,Q,P\}$, and then see whether Φ is invariant under $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$. The form of Φ and the invariance of Φ under $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$ depend on the form of $V(x)$.

In this note, we shall only consider potentials $V(x)$ that are bounded C^∞-functions with bounded derivatives. For such potentials, the maximal invariant subspace of the algebra $\{H,Q,P\}$ is the Schwartz space:

$$\Phi = \mathscr{S}(R)\,. \tag{23}$$

This space is indeed invariant under $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$, as the following theorem states for any dimension n [2]:

Theorem (Hunziker) *If $V(x)$ is a bounded C^∞-function on R^n with bounded derivatives, then $\mathscr{S}(R^n)$ is invariant under the unitary group $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$ and the mapping $(\varphi,t)\to \mathrm{e}^{-\mathrm{i}Ht/\hbar}\varphi$ of $\mathscr{S}(R^n)\times R$ onto $\mathscr{S}(R^n)$ is continuous (in the sense of the conventional topology of $\mathscr{S}(R^n)$).*

Thus, when $V(x)$ is a bounded C^∞-function with bounded derivatives, the time evolution (and therefore the Heisenberg picture) of the algebra $\{H,Q,P\}$ is well defined on $\Phi=\mathscr{S}(R)$. As a byproduct, the time evolution of the bras $\langle E|$, $\langle x|$, $\langle p|$ and kets $|E\rangle$, $|x\rangle$, $|p\rangle$ of H, Q, P is also well defined, since those bras and kets act as functionals over $\Phi=\mathscr{S}(R)$.

When $V(x)$ is not continuous but only piece-wise continuous (e.g., $V(x)$ is a rectangular barrier potential), the discontinuities of the potential have to be taken into consideration. For example, if $V(x)$ is continuous everywhere except at, say, $x=a,b$, then the maximal invariant subspace of $\{H,Q,P\}$ is the space $\mathscr{S}(R-\{a,b\})$ constructed in [1]. In this case, one has to prove that $\mathscr{S}(R-\{a,b\})$ is invariant under $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$. Although the invariance of $\mathscr{S}(R-\{a,b\})$ under $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$ is still to be proven, an examination of the proof of Hunziker's theorem [2] suggests that such invariance should hold.

For other "reasonable" potentials the invariance of the corresponding Φ under time evolution is to be expected, too. By "reasonable" we mean that the potential can be considered as a small perturbation to the kinetic energy, in the sense of Kato [3].

5. Conclusion

We have discussed the problems in defining the Heisenberg picture of an algebra of unbounded observables. We have seen that the Heisenberg picture is well defined when the maximal invariant subspace of the algebra remains invariant under the time evolution group. Such invariance should hold in general, although we have shown it only for potentials that are smooth. More precisely, when $V(x)$ is a bounded C^∞-function with bounded derivatives, Hunziker's theorem has been used to show that the Heisenberg picture of the algebra $\{H,Q,P\}$ is well defined on the Schwartz space.

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Note: The version of Hunziker's theorem I provided in this paper is not the most general one. In fact, after this paper was already in press, I realized that a theorem by Roberts [4] combined with the general version of Hunziker's theorem [2] guarantees that, when the potential is infinitely differentiable on some open set of R^n whose complement has zero Lebesgue measure, and when the potential satisfies the Kato condition [3], then the maximal invariant subspace of the algebra $\{H,Q,P\}$ is dense and invariant under $e^{-iHt/\hbar}$. In particular, the space $\mathscr{S}(R-\{a,b\})$ of [1] is indeed invariant under the time evolution of the 1D rectangular barrier Hamiltonian.

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