"AL.I.CUZA" UNIVERSITY

IASI

Department of Physics

ICEFIZ-
FT-155-1978 May

Substantiating problems of quantum mechanics

J.GOTTLIEB

Abstract : Some basic problems, related to the spaces and the operators necessary to describe quantum-mechanical phenomena, are entered upon from a new axiomatic standpoint. Some generalizations are operated, required by convergence criteria, concerning the Fourier transform, the Fourier product and the equation of eigen-values. Physical arguments are brought to support such generalizations and an analysis in view of organizing the structure of the proposed spaces is undertaken.

Dedicated to the 70-th birthday anniversary of Acad.Prof. ŞERBAN ŢIŢEICA

INTRODUCTION

In treating quantum mechanics, one usually starts with the probabilistic interpretation of the state function and, accordingly one postulates that the fundamental functional space, in which one operates within the discrete spectrum is the Hilbert space $L^2(R^3,C)$, which is the space of the square integrable complex functions of real variables.

Another fundamental postulate of quantum mechanics requires that :

$$\hat{x} = x \quad \text{and} \quad \hat{p}_x = \frac{1}{i}\frac{\partial}{\partial x}\ , \text{ with } \hbar = 1, \qquad (o.1)$$

should be operators acting on the state function (by means of circumflex we specify the operational character of these quantities). But the operators (o.1) cannot act but on a subset of L^2. Indeed, on one hand, not all the elements of L^2 are derivable, and on the other hand, from the assertion $f \in L^2$ does not necessarily result $\hat{x}f \in L^2$, as happens for instance in the case of the monodimensional function $f(x) = (x^2 + \alpha^2)^{-1/2}$ (α = constant).

Besides this contradiction, we mention also that the study of the continuous spectrum is characterized by a sensible degree of difficulty. It will suffice to mention O.M.Nikodym's papers [1] to illustrate this idea. Even the treatment based on "Gelfand's space triplet" [2] cannot solve the problem of continuous spectrum.

The fact that important mathematical specifications are necessary in dealing with quantum mechanics is also spotlighted in H.Triebel's treatise on higher analysis [3] .

The aim of the paper is to bring forth further specifications on functional spaces in which, we think, the mathematical formalism of quantum mechanics must be developed [4], [5]

1. THE FUNDAMENTAL FUNCTIONAL SPACE OF QUANTUM MECHANICS

To have at our disposal an adequate vocabulary, we shall call <u>wave function</u> any complex function of real variable that can be attached to a aprticle. When we deal with the discrete spectrum, we shall refer to the wave function as <u>state function</u>. We shall denote the set of wave functions by U and that of state functions by S.

As the wave functions satisfy linear and homogeneous differential equations and the principle of superposition does hold it results that :

A. *The set U forms a complex linear space*

But the same assertion is true for the state functions as well whence :

B. *The set S is a subspace of U*

Owing to the probabilistic interpretation, the state function must be an element of the Hilbert space L^2, therefore :

C. *S is a subspace of L^2*

For the sake of simplicity, we shall, before further specifications, consider complex functions of only one real variable .

Let $\mathcal{L}(S,S)$ be the space of the linear mappings (li -

near operators) $S \to S$, and $\mathcal{L}(U,U)$ the space of the linear mappings $U \to U$. From B. it follows that

D. $\mathcal{L}(U,U)$ is a subspace of $\mathcal{L}(S,S)$

In quantum mechanics it is assumed that

$$\hat{x} = x \in \mathcal{L}(U,U) \quad \text{and} \quad \hat{p} = -i\, d/dx \in \mathcal{L}(U,U). \tag{1.1}$$

Due to D. it is only natural to have

$$\hat{x} \in \mathcal{L}(S,S) \quad \text{and} \quad \hat{p} \in \mathcal{L}(S,S) \tag{1.2}$$

The condition for $\mathcal{L}(U,U)$, respectively $\mathcal{L}(S,S)$, to form a linear space of the linear mappings $U \to U$, respectively $S \to S$, is that

E. every entire function of $\hat{x}$ and $\hat{p}$ belongs to $\mathcal{L}(U,U)$, respectively $\mathcal{L}(S,S)$

*

* *

We have now provided all the data necessary for the specification of the contents of spaces U and S. But, before entering the very subject of the paper, we need still some definitions and denotations.

A function $f(x)$ on R is said to have the <u>asymptotic bound</u> $a(x)$ if and only if there exist two constants $K_1 > 0$ and $K_2 > 0$, so that for all $|x| > K_1$, the inequality $|f(x)| \leq K_2 a(x)$ does hold and we may write

$$f(x) = O(a(x)) \tag{1.3}$$

(In the case of functions of several variables the absolute value should be replaced by the Euclidian norm).

Let $f(x)$ be a continuous function and let us assume

$$f(x) = O(|x|^{\alpha}) , \qquad (1.4)$$

where α is a real constant. Then , we call f a *tempered function.*

We shall notice by C^{∞} the space of functions derivable as far as desired.

The function $f(x)$ of class C^{∞} is *rapidly decreasing* if for any $j \in N$ and $k \in N$(N is the set of natural numbers, 0 included) we have

$$\lim_{x \to \infty} |x^j f^{(k)}(x)| = 0 \qquad \text{with} \qquad f^{(k)} = d^k f/dx^k \qquad (1.5)$$

Tempered functions have the property that, together with f, both xf and the derivative of f (if there exist) are tempered functions. By corroborating this result with (1.1) we conclude that *it is likely to identify the space U with the space of tempered functions of class* C^{∞}.Due to ι.and (1.2) we shall identify the space S *with the space of rapidly decreasing functions*.

*

* *

We thinck we have to bring some specifications to the last statements.

One could object that wave functions are not always of class C^{∞}. This is true, but it is usually due to forced models (discontinuous variation of potential energy) and it only takes place on a set of null measure. In these instances (omitting those potentials of the type of infinite depth that do not approximate well any real case) the potential energy and wave function can be approximated as well as we want by functions of class C^∞. Thus, such examples can be maintained without contradicting our specifications on functional spaces of quantum mechanics.

Another objection might be due to the fact that the space S is not complete. Indeed, out of reasons of interpreting state functions, we consider S as a subspace of the Hilbert space L^2, hence endowed with a scalar product as in L^2 and with a norm induced by this scalar product. Let $f_n (n = 1,2,...)$ be a basis of S. It is also a basis of L^2 since S is dense in L^2 [7]. Any $f \in S$ can be written under the form

$$f = \sum_{n=1}^{\infty} c_n f_n \quad \text{with} \quad c_n \in C ,$$

where C is the field of complex numbers. The possibility of writing any state function under the form (1.6) is of particular interest in quantum mechanics. - On the other hand, not every convergent series in L^2 of the form (1.6) belongs to S, hence S has a pre-Hilbertian structure. But this does not prejudice the physical interpretations of the theory (the superposition principle refers to a finite number of states).

*

* *

Our oppinion is that only the limiting of the functional space of the state functions to the space S of the rapidly decreasing functions vindicates the famous polynomial method [8], [9].

2. FAMILIES OF WAVE FUNCTIONS

A characteristic representative for treating the continuous spectrum is the wave function of the free particle

$$\varphi(x,p) = e^{ipx}/\sqrt{2\pi} \; . \tag{2.1}$$

It stands for a family of functions belonging to U with the following important characteristics :

a) We have

$$\varphi(x,p)\Big|_{p=\text{const.}} \in U \quad \text{and} \quad \varphi(x,p)\Big|_{x=\text{const.}} \in U \tag{2.2}$$

b) To $\varphi(x,p)$ there corresponds an operator $\hat{\varphi}_x \in \mathcal{L}(S,S)$, or $\hat{\varphi}_p \in \mathcal{L}(S,S)$ via the relations

$$\begin{cases} \hat{\varphi}_x f = \int \varphi(x,p)\; f(p)\; dp = \tilde{f}(x) \in S \\ \hat{\varphi}_p f = \int \varphi(x,p)\; f(x)\; dx = \tilde{f}(p) \in S \; , \end{cases}$$

$\tilde{f}(x)$ and $\tilde{f}(p)$ respectively, being the Fourier transforms of $f \in S$.

c) The mapping of S on S given by $\hat{\varphi}_x$, or $\hat{\varphi}_p$, is continuous.

d) If $\hat{I}$ is the unit operator we have

$$\hat{\varphi}_p\, \hat{\varphi}_x = \hat{I} \; . \tag{2.4}$$

We say that $\hat{L} \in \mathcal{L}(S,S)$ is a <u>continuous mapping</u> if

$$\lim_{n\to\infty} f_n = 0 \qquad \text{implies} \qquad \lim_{n\to\infty} (\hat{L} f_n) = 0 \tag{2.5}$$

The necessary and sufficient condition for $\hat{L} \in \mathcal{L}(S,S)$ to be a continuous mapping is the existence of a number $M>0$ so that for any

$f \in S$ should have

$$\|\hat{L}f\| \leq M\|f\| \tag{2.6}$$

An operator satisfying (2.6) is called a <u>bounded</u> one. Thus, in the case of linear mappings, the set of continuous operators coincides with that of the bounded ones. These operators form a linear subspace $\mathcal{L}_c(S,S)$ of $\mathcal{L}(S,S)$. - According to (2.6), the space $\mathcal{L}_c(S,S)$ of the linear and continuous operators can be normalized by

$$\|\hat{L}\| = \sup_{\|f\| \leq 1} \|Lf\| \tag{2.7}$$

Now, let us prove that $\hat{\varphi}_x$ is a continuous mapping. From (2.1-4) we have

$$\begin{cases} \tilde{f}(x) = (2\pi)^{-1/2} \int e^{ipx} f(p)\, dp \\ f(p) = (2\pi)^{-1/2} \int e^{-ipx} \tilde{f}(x)\, dx \end{cases} \tag{2.8}$$

and

$$\begin{cases} \overline{\tilde{f}}(x) = (2\pi)^{-1/2} \int e^{-ipx} \bar{f}(p)\, dp \\ \bar{f}(p) = (2\pi)^{-1/2} \int e^{ipx} \overline{\tilde{f}}(x)\, dx \end{cases} \tag{2.9}$$

thus

$$\|\tilde{f}(x)\|^2 = \int \overline{\tilde{f}}(x)\, \tilde{f}(x)\, dx =$$

$$= (2\pi)^{-1/2} \int \overline{\tilde{f}}(x) \left[\int e^{ipx} f(p)\, dp \right] dx =$$

$$= \int \left[(2\pi)^{-1/2} \int e^{ipx} \overline{\tilde{f}}(x)\, dx \right] f(p)\, dp = \int \bar{f}(p)\, f(p)\, dp,$$

that is

$$\| \hat{\varphi}_x f \| = \| f \| \quad . \tag{2.10}$$

Comparing (2.10) to (2.6) there follows that $\hat{\varphi}_x$ is a bounded operator which means that it is a continuous one as well. Also, we find from (2.10) and (2.7) that

$$\| \hat{\varphi}_x \| = \| \hat{\varphi}_p \| = 1 \tag{2.11}$$

*

* *

Taking as a model the particular case of the free particle, we shall consider the set F of all the complex functions of two real variables $\chi(x,p)$ characterized by the fact that for every $f \in S$ the following relations are satisfied

$$\begin{cases} \chi(x,p)\Big|_{p=\text{const.}} \in U \quad \text{and} \quad \chi(x,p)\Big|_{x=\text{const.}} \in U \\ \hat{\chi}_x f = \int \chi(x,p)\; f(p)\; dp \in S \\ \hat{\chi}_p f = \int \chi(x,p)\; f(x)\; dx \in S \\ \hat{\chi}_x \in \mathcal{L}_c(S,S) \quad \text{and} \quad \hat{\chi}_p \in \mathcal{L}_c(S,S) \end{cases} \tag{2.12}$$

It is easy to remark that F is a linear space since together with $\chi_1, \chi_2 \in F$ we have $[c_1\chi_1 + c_2\chi_2] \in F$ with $c_1, c_2 \in C$.

The space F is very important in the study of the continuous spectrum. Therefore we will further suggest an adequate organization of this space.

We shall begin by proving that the adjoint operator of $\hat{x}_x$ is

$$\hat{x}_x^+ = \hat{\bar{x}}_p \tag{2.13}$$

Indeed, we have successively

$$(\hat{x}_x f, g) = \overline{(g, \hat{x}_x f)} =$$

$$= \overline{\int \bar{g}(x) \left[\int x(x,p)\ f(p)\ dp \right] dx} =$$

$$= \int \bar{f}(p) \left[\int \bar{x}(x,p)\ g(x)\ dx \right] dp =$$

$$= (f, \hat{x}_x^+ g) ,$$

where, (,) is the scalar product defined in S and in reverting the integration order we used Fubini's theorem [10]*)

Now, we shall define a mapping $F \times F \to \mathcal{L}_c(S,S)$, that we shall call Fourier product and denote it with $(\ , \ )_F$, by

$$(x_1(x,p'),\ x_2(x,p))_F = \hat{L} \in \mathcal{L}_c(S,S) \quad , \tag{2.14}$$

with

$$\hat{L}f = \int \bar{x}_1(x,p') \left[\int x_2(x,p)\ f(p)\ dp \right] dx \quad . \tag{2.15}$$

Relation (2.15) can also be written in the form

$$\hat{L} = \hat{\bar{x}}_{1p}, x_{2x} \quad , \tag{2.16}$$

or, taking into considerations (2.13),

$$\hat{L} = \hat{x}_{1x}^+\ \hat{x}_{2x} \quad . \tag{2.17}$$

---

*) $\iint \bar{f}(p)\ \bar{x}(x,p) g(x) dx\ dp = \iint \bar{f}(x) \bar{x}(p,x) g(p)\ dp\ dx$

$= \iint \bar{f}(x) \bar{x}(x,p) g(p)\ dp\ dx$, because $x(x,p) = x(p,x)$

The Fourier product thus defined has characteristics similar to those of the scalar product, namely

$$\begin{cases} (\chi(x,p'),\chi(x,p))_F = \hat{L}_o, \quad \text{with } (f,\hat{L}_o f) \geqslant 0 \quad \forall\, f \in S \\ (\chi_1(x,p'),\chi_2(x,p))_F^+ = (\chi_2(x,p'),\chi_1(x,p))_F \\ (\chi_1 + \chi_2,\chi)_F = (\chi_1,\chi)_F + (\chi_2,\chi)_F \\ (\chi_1, c\chi_2)_F = c(\chi_1, \chi_2)_F , \quad \forall\, c \in C . \end{cases} \tag{2.18}$$

Let us verify these relations. From (2.17) we have

$$(f, \hat{L}_o f) = (f, \hat{\chi}_x^+ \hat{\chi}_x f) = (\hat{\chi}_x f , \hat{\chi}_x f) \geq 0 ,$$

and this justifies (2.18.1) . Similarly, from (2.13) and (2.16) it follows

$$(\chi_1(x,p'), \chi_2(x,p))_F^+ = (\hat{\hat{\chi}}_{1p}, \hat{\chi}_{2x})^+ = \hat{\chi}_{2x}^+ \hat{\bar{\chi}}_{1p}^+ =$$

$$= \hat{\hat{\chi}}_{2p}, \hat{\chi}_{1x} = (\chi_2(x,p').\chi_1(x,p))_F ,$$

thus relation (2.18.2) is a' , true. The equalities (2.18.3) and (2.18.4) verify easily taking into account the definition (2.15) of the Fourier product.

*

* *

As the space $\mathscr{L}_c(S,S)$ is normalized by (2.7), the Fourier product induces a norm in F by

$$\| \chi(x,p) \| = \| \hat{L}_o \|^{1/2} , \tag{2.19}$$

with $\hat{L}_o$ given by (2.18.1). Thus F becomes a normalized space, which is of particular interest in the treatment of the continuous spectrum in quantum mechanics.

*

* *

The function $\psi(x,p)\in F$, which satisfies also the relation (2.4), namely

$$\hat{\bar{\psi}}_p \hat{\psi}_x = \hat{I} , \qquad (2.20)$$

plays an important role. As a matter of fact, using the denotations to be found in treatises of physics, this relation assumes the form

$$\int \bar{\psi}(x,p')\psi(x,p)\, dx = \delta(p'-p) , \qquad (2.21)$$

δ being the Dirac generalized function.

From (2.19) and (2.20) we get

$$\|\psi(x,p)\| = \|\hat{\bar{\psi}}_p \hat{\psi}_x\|^{1/2} = \|\hat{I}\|^{1/2} = 1 \qquad (2.22)$$

Thus, these functions will play the role of normalized eigen - functions of the operators of quantum mechanics in the case of the continuous spectrum.

The function $\psi(x,p)$ with the property (2.20) allows <u>the generalization of the Fourier transform</u> in the form

$$\tilde{f}_\psi(x) = \int \psi(x,p)\, f(p)\, dp \in S \quad . \qquad (2.23)$$

Owing to (2.20) there exists the inverse transform, and we have

$$f(p) = \int \bar{\psi}(x,p)\, \tilde{f}_\psi(x)\, dx . \qquad (2.24)$$

3. *OPERATORS*

The Fourier product allows the generalization of some definitions in the theory of operators. Indeed, let $\mathcal{L}(F,F)$ be the space of linear mappings $F \to F$. If $\hat{A} \in \mathcal{L}(F,F)$ and there exists a $\hat{A}^+ \in \mathcal{L}(F,F)$ so that for any $[\chi_1, \chi_2] \in F$ we have

$$(\chi_1(x,p'),\ \hat{A}^+ \chi_2(x,p))_F = (\hat{A}\chi_1(x,p'),\ \chi_2(x,p))_F \quad , \tag{3.1}$$

then $\hat{A}^+$ is the <u>Hermitian conjugate of $\hat{A}$</u>. If

$$\hat{A}^+ = \hat{A} \tag{3.2}$$

then $\hat{A}$ is a <u>Hermitian operator</u>.

The operator $-i\partial/\partial x$ is Hermitian. Indeed, let

$$\hat{p}^+ = -i\partial/\partial x \ . \tag{3.3}$$

Then

$$(\chi_1(x,p'),\ \hat{p}^+\chi_2(x,p))_F f = \int \bar{\chi}_1(x,p')[\int \frac{1}{i}\frac{\partial}{\partial x}\ \chi_2(x,p')f(p)dp]dx =$$

$$= \int \bar{\chi}_1(\ ,p')\ \frac{1}{i}\frac{d}{dx}\ \phi(x)\ dx \quad ,$$

where we denoted

$$\phi(x) = \int \chi_2(x,p)\ f(p)\ dp \in S \quad .$$

Thus

$$(\chi_1(x,p'),\ \hat{p}^+\chi_2(x,p))_F f =$$

$$= -i\chi_1(x,p')\phi(x)\Big|_{-\infty}^{+\infty} + \int i[\partial\chi_1(x,p')/\partial x]\ \phi(x)dx =$$

$$= \int \overline{-i\partial\chi_1(x,p')/\partial x}[\int \chi_2(x,p)\ f(p)\ dp]dx =$$

$$= (-i\partial\chi_1(x,p')/\partial x,\ \chi_2(x,p))_F f \quad .$$

whence $\hat{p}^+ = \hat{p}$, as was expected.

It can be proved that if for an operator $\hat{A}$ there exists

$\hat{A}^+$, then the latter is unique [5] .

*

* *

We may consider the set of functions in F still as a subspace of U, where $\chi(x,p)$ is a family of functions pertaining to U, and p is a parameter. Let $\hat{L}\in\mathcal{L}(U,U)$ be an operator for which F is an invariant subspace. Then, we also have $\hat{L}\in\mathcal{L}(F,F)$ but $\hat{L}$ operates only on the x variable of $\chi(x,p)$ through the relation

$$\hat{L}\left[\chi(x,p)\Big|_{p=p_0}\right] = \left[\hat{L}\,\chi(x,p)\right]\Big|_{p=p_0} , \qquad (3.4)$$

which holds for every fixed but arbitrary p_0. The operator $\hat{p}$, defined by (3.3) is such an operator. Further on, we shall deal with such operators.

We shall generalize the equation of eigenvalues and eigenfunctions under the form

$$\hat{L}\chi(x,p) = \alpha(p)\chi(x,p) , \qquad (3.5)$$

where $\alpha(p)\in U$. We also have some results similar to those known in the theory of operators from $\mathcal{L}(L^2,L^2)$. Thus, <u>if $\hat{L}$ is Her - mitian, the function $\alpha(p)$ is real</u>. Indeed, from (3.1) we obtain:

$$(\chi(x,p'),\ \hat{L}\chi(x,p))_F = (\hat{L}\chi(x,p'),\chi(x,p))_F$$

and substituting here (3.5) there results

$$(\chi(x,p'),\alpha(p)\chi(x,p))_F = (\alpha(p')\chi(x,p'),\chi(x,p))_F . \quad (3.6)$$

Taking into account (2.15) , this means that for any $f\in S$ we should have

$$\int \bar{\chi}(x,p')\left\{\int [\alpha(p) - \bar{\alpha}(p')]\ \chi(x,p) f(p)\ dp\right\} dx = 0 \ . \qquad (3.7)$$

As f(p) is arbitrary, for a fixed p' we shall choose it as a function whose support is the neighbourhood $(p'-\varepsilon,\ p'+\varepsilon)$ of p'. As $\varepsilon>0$ is arbitrary, from (3.7) there results

$$\alpha(p') = \bar{\alpha}(p') \ , \qquad (3.8)$$

thus $\alpha(p)$ is a real function.

If we suppose that $\alpha(p)$ is a monotone function, while p' is fixed, then, also from (3.7) it results that

$$(\chi(x,p'),\ \chi(x,p))_F$$

is a distribution whose support is only one point , namely $p=p'$. But ([6] , p.35) a distribution whose support is only one point, is a finite linear combination of Dirac's δ-function and its derivatives. Beside this, let us also take into account the fact that in a small enough neighbourhood of p we can put

$$\alpha(p) - \alpha(p') = a(p - p') \qquad (a = \text{const.})$$

and therefore we must have for our distribution

$$(\chi(x,p'),\ \chi(x,p))_F\, \delta(p-p') = 0$$

Therefore, we infer the relation

$$(\chi(x,p'),\ \chi(x,p))_F = \beta(p)\ \delta(p'-p) \qquad (3.9)$$

and, accordingly, the quantitites

$$\psi(x,p) = (\beta(p))^{-1/2}\ \chi(x,p) \qquad (3.10)$$

are eigenfunctions of $\hat{L}$ and the norm of the family $\psi(x,p)$ is equal to 1.

Now, it becomes obvious that for the operator $\hat{p}=-i\partial/\partial x$ we have

$$\hat{p}\varphi(x,p) = p\,\varphi(x,p) \quad , \tag{3.11}$$

with

$$\varphi(x,p) = e^{ipx}/\sqrt{2\pi} \tag{3.12}$$

and

$$\|\varphi(x,p)\| = 1 \; . \tag{3.13}$$

*

* *

The above mentioned problems allow a more unitary treatment of the discrete spectrum and of the continuous one. Supposing that any wave function depends on x,y,z,t and for every coordinate it satisfies a normalized relation (either of the discrete spectrum or of the continuous one), the temporal dependence gains the same right as the spatial ones, just as it is imposed in E.Schmutzer's valuable paper [11] .

R E F E R E N C E S

[1] O.M.Nikodým , The Mathematical Apparatus of Quantum Theories, Springer Verlag, Berlin - Heidelberg - New York, 1966.

[2] I.M.Gelfand, N.J.Wilenkin, Verallgemeinerte Funktionen IV, VEB, Berlin 1964.

[3] H.Triebel, Höhere Analysis, VEB, Berlin 1972.

[4] J.Gottlieb, On the Functional Spaces of Quantum Mechanics - Preprint Univ.Timişoara, UTFT-5/09/1976.

[5] J.Gottlierb, T.Jucan, R.T.Vescan, P.Iacob, On a Class of Fourier-Type Integral Transforms - An.şt.Univ.Iaşi (s.n.), Sect.Ia., Tom XXIII, p.391.

[6] H.Bremermann, Distributions, Complex Variables and Fourier Transforms, Addison-Wesley Publ.Comp., Inc., Mass., 1965.

[7] L.Hörmander, Linear Partial Differential Operators , Springer Verlag, Berlin-Gottingen-Heidelberg, 1963, p.37.

[8] E.Schrödinger, Quantisierung als Eigenwertproblem I, Ann. der Phys. (4), 79 , 1926, p.361.

[9] A.Sommerfeld, Atombau und Spektrallinien. Wellenmechanischer Ergarzband, Vieweg, Braunschweig, 1929.

[10] M.Nicolescu, Funcţii reale şi elemente de analiză funcţională, Ed.Did. şi Ped.Bucureşti, 1962, p.145.

[11.] E.Schmutzer, Eine neue Grundlegung der Quantentheorie, Nova Acta Leopoldina, 44, Nr.8, Suppl., 1976, p.79.