Hilbertian structure of quantum physics and Schrödinger operators

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Abstract

Schrödinger operators are a specific class of linear operators, acting in a separable Hilbert space over the field $\mathbb{C}$, that arise from quantum physics. Here we try to explain how non-relativistic quantum physics is characterized by a Hilbert space structure. Then we discuss the particular physical system consisting in an elementary quantum particle[1], which leads to Schrödinger operators.

1 Hilbertian structure of quantum physics

There are two suitable approaches to "endow" quantum mechanics with a Hilbert space structure. The first is based on a lattice-theoretical formulation of the properties of a quantum system, the so called propositional calculus of quantum mechanics. The second consists in an algebraic formulation of quantum mechanics extending the von Neumann synthesis of the quantum theories of Heisenberg, Born and Jordan (matrix mechanics – 1925), and Schrödinger (wave mechanics – 1926). In the latter approach there is a "direct" Hilbert space formulation of quantum mechanics [vN46]. Here we will deal only with *pure quantum systems* (but both approaches apply in a more general context).

The main idea of the propositional calculus of quantum mechanics is that a physical system can be described in term of so called "*yes-no experiments*". The latter are tests on the systems which permit only one of two alternatives as an answer. We define a *proposition* as a property of the system tested by an equivalence class of physical "yes-no experiments" (all the elements in the same equivalence class test the same property). Moreover the system exists independently of our knowledge of its propositions, and we investigate the *properties of the propositions* of a physical system which are *independent of the state* of the system.
The set of all propositions of a physical system is supposed to have the mathematical structure of a complete orthocomplemented lattice $\mathcal{L}$. This means that $\mathcal{L}$ is a partially ordered set, that each subset of $\mathcal{L}$ admits a greatest lower bound and a smallest upper bound and that there exists an orthocomplementation. The structure of this lattice is independent of the state of the physical system, in others

[1]See below for the definition of elementary quantum particle.

words $\mathcal{L}$ describes the *intrinsic structure* of the system.
As an example of "yes-no experiment", consider a particle in $\mathbb{R}^d$. A "yes-no experiment" is, for example, a test T_Δ on the particle (realized with a particle counter located in Δ) that has the answer "yes" if the particle is detected in a given subset $\Delta \subset \mathbb{R}^d$ and "no" otherwise. Denote by P_Δ the proposition (in $\mathcal{L}$) associated to T_Δ. P_Δ is "*true*" if the answer is "yes" with *certitude* (all repetitions of the experiment always yields the same result or equivalently the answer "no" is impossible) and "*not true*" otherwise. Clearly if $\Delta' \subset \Delta''$, whenever the response to $T_{\Delta'}$ is "yes", the response to $T_{\Delta''}$ must also be "yes". Therefore there exists a relation between certain pairs of propositions : if $P_{\Delta'}$ is "true" then $P_{\Delta''}$ must be "true" ($\mathcal{L}$ is partially ordered). Moreover, to the proposition $P_\Delta \in \mathcal{L}$ corresponds the orthocomplemented proposition $P_\Delta^{'} \in \mathcal{L}$ tested by T_{Δ^c} ($\Delta^c = \mathbb{R}^n \backslash \Delta$). In this case, if P_Δ is "true", then $P_\Delta^{'}$ is "*false*" (distinguished *in general* from "not true"), and viceversa.
Under five axioms, $\mathcal{L}$ can be represented as the set of all closed subspaces of a separable complex Hilbert space $\mathcal{H}$, denoted by $\mathcal{P}(\mathcal{H})$.
$\mathcal{P}(\mathcal{H})$ has clearly the structure of a complete orthocomplemented lattice, where the orthocomplemetation is the orthogonal $^\perp$ in the usual sense of the "geometry" of Hilbert spaces.
Each proposition corresponds to one of such closed subspaces, or equivalently to an orthogonal projector on $\mathcal{H}$ (bijection between $\mathcal{P}(\mathcal{H})$ and the orthogonal projectors on $\mathcal{H}$). In this framework *observables* are represented by spectral measures or equivalently, via the Spectral Theorem [RS72, Thm. VIII.6], as self-adjoint operators. The *states* are represented by the self-adjoint positive trace class operators ρ with $\mathrm{Tr}\,\rho = 1$. In particular the pure states of the system correspond to the one-dimensional projectors, or equivalently the closed one dimensional subspaces of $\mathcal{H}$ (the atoms of the lattice $\mathcal{P}(\mathcal{H})$) [Jau68], [Pir90], [RS98].

We now switch to the C^*−algebraic approach, following [Emc84, Chap. 9]. The fundamental postulate in this approach is the C^*−algebraic postulate: A physical system is characterized by a triple $\{\mathcal{E}, \mathcal{A}, \langle\cdot;\cdot\rangle\}$ where: $\mathcal{A}$, the set of its *observables*, is the collection of all the self-adjoint elements A of a C^*−algebra $\mathcal{B}$ with identity I; $\mathcal{E}$, the set of its *states*, is the collection of all real-valued, positive linear functionals ρ on $\mathcal{A}$, normalized by the condition $\langle \rho, I\rangle = 1$; and $\langle\cdot;\cdot\rangle$ is the prediction rule which attributes, to every pair $(\rho, A) \in \mathcal{E} \times \mathcal{A}$, the value $\langle \rho; A\rangle$ of ρ at A, interpreted as the expectation of the observable A when the system is in the state ρ.
When we deal with a quantum system the C^*−algebra $\mathcal{B}$ is non-commutative and can be represented as a non-commutative subalgebra of the algebra of bounded linear operators on a Hilbert space [Dix69, Thm. 2.6.1]. That is, there exists an abstract Hilbert space $\mathcal{H}$ and an injective map $\pi : \mathcal{B} \longrightarrow \mathcal{L}(\mathcal{H})$ ($\mathcal{L}(\mathcal{H})$ is the C^*−algebra of bounded linear operators on $\mathcal{H}$) that is an algebraic $*$−homomorphism. In this framework the elements of $\mathcal{E}$ can be represented as density matrices, and pure states as one dimensional projectors, that are equivalence classes of vectors in $\mathcal{H}$.

We see that in both cases one can put a Hilbertian structure on a quantum system. But until now we only know that *there exists* an *abstract Hilbert space* $\mathcal{H}$, that observables are represented as self-adjoint operators acting in $\mathcal{H}$, that pure states are represented as rays in $\mathcal{H}$ and mixed states as positive self-adjoint operators with trace one (density matrices). Below we sketch to show how we can get a concrete realization of the abstract Hilbert space for one of the simplest physical systems.

2 Elementary quantum particle

We consider a *special physical system*: a (quantum) elementary particle in the configuration space $\mathbb{R}^d$, $d = 2, 3$ (without spin). The quantum elementary particle is the analogous of the classical point particle, in the sense that it is the simplest system for which at each time t two *observables* are defined: the *position* and the *momentum*. In this context, the word "elementary" means that there are no other non-trivial observables which are independent of the position and the momentum.

The problem is to give a concrete realization of the abstract Hilbert space for this physical system. To do this we need to consider the basic properties of physical space: its *homogeneity* and its *isotropy*. Both of these properties express the fact that the physical space has no observable physical properties: different points in the physical space are physically indistinguishable.
Consider first the observable position. The key concept is the *localisability* of the particle in some (Borel) subset Δ of the configuration space $\mathbb{R}^d$. To each $\Delta \in \mathcal{B}(\mathbb{R}^d)$ we associate a closed subspace $\mathcal{E}_\Delta \in \mathcal{P}(\mathcal{H})$, or equivalently an orthogonal projector E_Δ. We assume that the map $\mathcal{B}(\mathbb{R}^d) \longrightarrow \mathcal{P}(\mathcal{H})$ is a $\sigma-$homomorphism, that is an observable (see [Jau68, p.98]). The Borel sets Δ are subsets of $\mathbb{R}^d$ and the projectors E_Δ are projectors representing the "yes-no experiments" corresponding to find the particle in the subset Δ.
By space translations ($x \mapsto x + \alpha$) and rotations ($x \mapsto Rx$) we can associate to each Δ a subset $(R, \alpha) \circ \Delta := R\Delta + \alpha$. The set of all (R, α) forms the group of motions of $\mathbb{R}^d$. Space homogeneity and space isotropy imply that translations and rotations are symmetries of the system and lead to the condition $\mathcal{E}_{(R,\alpha)\circ\Delta} = U(R, \alpha)\mathcal{E}_\Delta$ (or equivalently $E_{(R,\alpha)\circ\Delta} = U(R, \alpha)E_\Delta U(R, \alpha)^{-1}$), where, by the Wigner Theorem [Amr98], $U(R, \alpha)$ is a (projective) representation of the group $\{(R, \alpha)\}$ of motions of $\mathbb{R}^d$. This leads to the following commutative diagram, called *system of imprimitivity* for the position

$$\begin{array}{ccc} \mathcal{B}(\mathbb{R}^d) \ni \Delta & \longrightarrow & \mathcal{E}_\Delta \in \mathcal{P}(\mathcal{H}) \\ \downarrow{\scriptstyle (R,\alpha)} & & \downarrow{\scriptstyle U(R,\alpha)} \\ \mathcal{B}(\mathbb{R}^d) \ni (R, \alpha) \circ \Delta & \longrightarrow & \mathcal{E}_{(R,\alpha)\circ\Delta} = U(R, \alpha)\mathcal{E}_\Delta \in \mathcal{P}(\mathcal{H}) \end{array} .$$

A similar system of imprimitivity can be written for the momentum observable. To each $\Omega \in \mathcal{B}(\mathbb{R}^d)$ in the "momentum" space we associate a closed subspace $\mathcal{F}_\Omega \in \mathcal{P}(\mathcal{H})$, or equivalently an orthogonal projector F_Ω. The group symmetry is here that of momentum translations ($p \mapsto p + w$) and momentum rotations ($p \mapsto Rp$) (R is the same as for the position, since the classical direction of the momentum and position vectors refers to the configuration space).

$$\begin{array}{ccc} \mathcal{B}(\mathbb{R}^d) \ni \Omega & \longrightarrow & \mathcal{F}_\Omega \in \mathcal{P}(\mathcal{H}) \\ \Big\downarrow {\scriptstyle (R,w)} & & \Big\downarrow {\scriptstyle U(R,w)} \\ \mathcal{B}(\mathbb{R}^d) \ni (R,w)\circ\Omega & \longrightarrow & \mathcal{F}_{(R,w)\circ\Omega} = U(R,w)\mathcal{F}_\Omega \in \mathcal{P}(\mathcal{H}) \end{array} .$$

From the theory of the systems of imprimitivity, we can prove that the above imprimitivity systems determine completely the model of the elementary quantum particle. This determination is up to unitary equivalence and to an arbitrary parameter denoted by $\hbar$ [Pir90], [Jau68], [RS98].
The results are: the *Hilbert space* is $\mathcal{H} = L^2(\mathbb{R}^d, \mathrm{d}x)$. The *unitary representations* act on $\psi \in L^2(\mathbb{R}^d)$ as $[U_\alpha \psi](x) = \psi(x-\alpha)$, $[U_w\psi](x) = e^{i\,x\cdot w/\hbar}\psi(x)$ and $[U_R\psi](x) = \psi(R^{-1}x)$, and satisfy the *Weyl relations* $U_w U_\alpha = e^{iw\cdot\alpha/\hbar}U_\alpha U_w$. The *position operator* X acts as $(X\psi)(x) = x\psi(x)$, while the *momentum operator* P acts as $(P\psi)(x) = (-i\hbar\nabla\psi)(x)$. X and P are essentially self-adjoint on $C_0^\infty(\mathbb{R}^d)$ and satisfy the *Heisenberg canonical commutation relations* $[X_k, P_\ell] = i\hbar\delta_{k\ell}I$ defined on a dense set of vectors in $L^2(\mathbb{R}^d)$. P is the infinitesimal generator of the space translations $U_\alpha = e^{-i\alpha\cdot P/\hbar}$ and X is the infinitesimal generator of the momentum translations $U_w = e^{iw\cdot X/\hbar}$.

We are interested in the dynamical structure of our physical system consisting in a quantum particle. The dynamical structure contains the law which governs the time evolution of the states. We shall assume that we are dealing with a *conservative system.* Such systems interact with the external world only through constant forces (no time dependence) and do not react back on this world at all. We suppose that the state at one instant of time determines uniquely the state at any other time and that this transformation of states is *continuous.* In other words we suppose that the *time evolution* is *deterministic* (as it is in classical mechanics). Finally, we also suppose *homogeneity of time*, or equivalently that time evolution is a symmetry transformation of the system.
According to the hypothesis above the time evolution is described by a group homomorphism which maps the real line continuously to a one-parameter group of unitary operators acting in $\mathcal{H}$ (Wigner Theorem). The homomorphism $t \longrightarrow U_t$ is called the *dynamical* (*or evolution*) *group* of the system. Consider at time $t = 0$ that the system is in a pure state given by a vector $\psi_0 \in \mathcal{H}$, then the state at time t is given by the vector $\psi_t = U_t\psi_0$.
We now look at the infinitesimal generator of the dynamical group $\{U_t\}_{t\in\mathbb{R}}$. The set of vectors $\psi \in \mathcal{H}$ for which

$$\text{s-lim}_{t\to 0} \tfrac{i\hbar}{t}\,[U_t - I]\psi = H\psi$$

exists is the domain $\mathcal{D}(H)$ of a *self-adjoint* operator H as defined above, moreover $\mathcal{D}(H)$ is dense in $\mathcal{H}$ (Stone Theorem [RS72, Thm. VIII.8]). H is called the *Hamiltonian*, it generates the dynamics of the system and it represents the energy observable of the system.

It remains to determine the form of the Hamiltonian. For this we need to introduce the *velocity*. It is defined as the formal differentiation of the position operator in the Heisenberg picture (at $t = 0$): $\dot{X} = \frac{i}{\hbar}[H, X]$. From the latter equation it follows that if we impose certain properties on $\dot{X}$, we must expect that they will restrict the possibilities for H. We will impose the *principle of Galilei invariance*, meaning that the Galilei transformations $X \longrightarrow X$ and $\dot{X} \longrightarrow \dot{X} + v$ are symmetries for the system (in classical mechanics these transformations leave the equations of motion invariant). One can prove (using Weyl relations) that the unitary group associated to this transformation is $W_v = e^{-i\,m\,v\cdot X/\hbar}$, with m a parameter [Jau68]. Thus

$$W_v \dot{X} W_v^{-1} = \dot{X} + v \qquad \text{and also} \qquad \frac{1}{m} W_v P W_v^{-1} = \frac{P}{m} + v\ .$$

Taking the difference and considering the form of W_v it follows that $m\dot{X} = P - A(X)$. Then, by the canonical commutation relations, $m[X_k, \dot{X}_\ell] = i\hbar\delta_{k\ell}I$, it follows that the operator $H_0 = \frac{m}{2}\dot{X}^2$ satisfies $\frac{i}{\hbar}[H_0, X] = \dot{X}$. We can thus conclude that the most general form of H is

$$H = \frac{(P - A(X))^2}{2m} + V(X) \tag{$\star$}$$

where m is interpreted as the particle mass. The identification of m with the particle mass follows if we identify the classical motion of the particle with the motion of the expectation value of the position operator. V represents an external potential and A represents a gauge field that is identified with a vector potential associated to an external magnetic field (more precisely we identify it with $\frac{1}{q}A$, q being the electric charge of the particle).
The aim of this discussion was to motivate our interest in the study of this specific class of self-adjoint operators given by (non relativistic) Hamiltonian operators of the form ($\star$) acting on the Hilbert space $L^2(\mathbb{R}^d)$, the so called *Schrödinger operators*. Of course, the form of $A(X)$, $V(X)$ and the dimension d of the configuration space depend on the specific physical model under consideration.

References

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