Physical Framework of Quantization Problem

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Abstract: The paper presents shortly the geometric approach to the problem of a general quantization formalism, both physically meaningful and mathematically consistent.

Key words: old quantum mechanics, geometric quantization.

The notion of quantization has appeared at the beginning of the century in the theory of heat radiation, since M. Planck has formulated the hypothesis of the energy quanta [1]. This hypothesis assumed a finite number of ways to distribute the energy of the \( \nu \)-frequency radiation over a given number of oscillators, every distribution assigning to each oscillator integer multiples of the "energy quantum" \( \epsilon = h\nu \), \( h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s} \). Later on, the Planck's hypothesis was interpreted as a consequence of a "quantum constraint" acting in general on the harmonic oscillator considered as classical system. Thus, the problem of quantization was to "select an infinite, discrete number of quantum possible real motions, from the continuous manifold of all mechanically possible motions" [2], by an appropriate system of constraints. The action of these constraints on the classical motion as a whole, and not on the physical state at a given time, has suggested to express them as restrictions on the geometrical quantities associated with the trajectory in the space of the classical states. These states were identified with the points of the phase space, locally parameterized by generalized coordinates and momenta. The dimensional equality between the constant \( h \) and the classical action has allowed to select the quantum trajectories for the separable systems with multiple periodic motions by using the conditions of Bohr, Wilson and Sommerfeld (BWS), requiring the phase integrals \( J_k = \oint p_k dq^k \), \( k = 1, 2, ..., n \), (\( n \) is the number of freedom degrees) to be integer multiples of

\(^1\)first printed as preprint 102-(1990) by the University of Timisoara, Romania.
the "action" quantum $h$:

$$J_k = \oint p_k dq^k = n_k h, \quad n_k = 0, 1, 2, ...$$  \hfill (1)

Because $p_k$ is given by the solution $S(q^1, q^2, ..., q^n, \alpha_1, \alpha_2, ..., \alpha_n)$ of the Hamilton-Jacobi equation:

$$H(\frac{\partial S}{\partial q}, q) = \alpha_1 ,$$  \hfill (2)

$$\frac{\partial S}{\partial q} \equiv \{ \frac{\partial S}{\partial q^1}, ..., \frac{\partial S}{\partial q^n} \}, \quad q \equiv \{ q^1, q^2, ..., q^n \},$$

as $p_k \equiv \frac{\partial S}{\partial q^k}$, the condition (1) selects a discrete set of integration constants $\{ \alpha_1, \alpha_2, ..., \alpha_n \}$ corresponding to the quantum allowed motions.

The application of these quantization formulas has led to a description in agreement with the experiment for the energy levels of the hydrogen atom, or for the Stark and Zeeman effects. Also, by quantizing the relativistic Kepler problem, the fine structure of the spectral lines was explained.

Besides its success, the method of phase integrals quantization was faced with various shortcomings, and in particular it was not able to give a quantum description for the free micro-particles. In 1924 Louis de Broglie has formulated the principle of duality, extending the double nature of light, as wave and particle, to all forms of matter. So, to a free micro-particle without spin, having the energy $E = mc^2, \quad m = m_0/\sqrt{1 - v^2/c^2}, \quad m_0 =$ the rest mass, a scalar plane wave having the frequency $\nu = E/h$, the wavelength $\lambda = h/mv$ and the group velocity $v_g = \frac{d\omega}{dk} = \frac{dE}{d(mv)} = v$, was associated.

The wave associated to the micro-particles placed in potential force fields was obtained by extending the correspondence between the geometrical and wave optics. Within the geometrical optics, the way of the light rays may be equivalently described by the wave surfaces $S(x, y, z) =$ constant, orthogonal to the rays. The equation determining the function $S$ is formally identical with the Hamilton-Jacobi equation, and it can be obtained from the wave equation written for monochromatic waves in the limit of small wave-lengths. This correspondence, together with de Broglie’s formulas for the free particle, has suggested a "kinematic" quantization, by expressing the refraction index from the monochromatic waves equation through the classical potential energy. The final equation obtained for the wave function $\Psi$, written as

$$\Delta \Psi + \frac{2m}{\hbar^2} (E - V) \Psi = 0, \quad \hbar = \frac{h}{2\pi},$$  \hfill (3)
with $E$ and $V$ the total and the potential energy, respectively, has accurately solved the problem of the energy spectra for all the potentials known as physically relevant.

Intending to establish a dynamical equation, able to describe the time-evolution of the micro-particles, the equation (3) was generalized, but the result was proved to be a breakdown with the classical wave picture. Thus, by contrast to the classical equation for real waves, the fundamental quantum dynamical equation:

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (4)$$

contains only the first order time-derivatives of $\Psi$. This equation can be found by acting on $\Psi$ with the operator equation resulting when the derivatives $p = \frac{\partial S}{\partial q}$, $s = -\frac{\partial S}{\partial t}$ from the time-dependent Hamilton-Jacobi equation $H(p, q, t) = -s$, are replaced by the operators $\hat{p} = -i\hbar \frac{\partial}{\partial q}$, $\hat{s} = -i\hbar \frac{\partial}{\partial t}$, but in general the non-commutativity of $\hat{p}$ and $q$ leads to ambiguities in the definition of the operator $\hat{H}$. Consequently, the further line of reasoning was to take the dynamics of $\Psi$ as basically independent on a underlying classical picture, and to see the correspondence between the operator $\hat{H}$ and the classical Hamilton function $H(p, q, t)$, if any, merely as an accident. Within the new formulation, known as quantum mechanics, the function $\Psi$ is not an observable, and moreover, it is not a wave in the usual three-dimensional space, but it is a representative element for the "quantum state" of the system. This state is a ray in an abstract Hilbert space $H$, without any classical correspondent, associated to the quantum system. Its dynamics is determined by the time-dependent Schrödinger equation (4), where $\hat{H}$ is a self-adjoint operator defined on a dense domain in $H$. Because the rays of $H$ and the operators on $H$ are not observables, the "quantization problem" was apparently eliminated, but in fact it was shifted towards the connection with the experiment. Before analyzing more closely this problem, it is interesting to remark that even the fundamental quantum equation (4) contains a variable considered to be classically defined, namely the time $t$. More generally, the whole space-time framework is classical, and all the observables are classical quantities, subject to classical dynamics.

Defining the value of an observable in a given state $\Psi$ as the mean-value $\langle \Psi | \hat{A} | \Psi \rangle$ of a symmetric operator $\hat{A}$ which is associated to the observable, the kinematic task of the quantization problem was to construct the Hilbert space $H$ and the correspondence between observables and operators. To ob-
tain this correspondence, Dirac (1930) has suggested an algebraic method based on the construction of an isomorphism between the Lie algebra of the operators on $\mathcal{H}$ and the Poisson algebra of the observables [3]. Considering the set of observables be represented by the set $\mathcal{F}(M)$ of the smooth real functions over a classical phase space $(M, \omega)$, with $\omega$ the globally defined symplectic form, then it becomes a Lie algebra defining the Poisson bracket $\{\cdot, \cdot\}$ by:

$$\{f, g\} = \omega(X_f, X_g) = L_{X_f}g, \quad f, g \in \mathcal{F}(M) .$$

(5)

Here $X_f$ is the vector field determined by $i_{X_f}\omega = df$, and $L_{X_f}$ denotes the Lie derivative with respect to $X_f$. In the case when $M = T^*Q$, $Q = R^n$, the symplectic form is $\omega_0 = \sum_{k=1}^n dp_k \wedge dq_k$, and the complete quantization of $Q$ was defined as an $R$-linear map $f \rightarrow \hat{f}$ from $\mathcal{F}(M)$ to a set $\mathcal{A}(\mathcal{H})$ of symmetric operators on the Hilbert space $\mathcal{H}$, having the following properties [4]:

1. the map $\hat{\cdot} : \mathcal{F}(M) \rightarrow \mathcal{A}(\mathcal{H})$ is injective.
2. $[\hat{f}, \hat{g}] = i\hbar \{f, g\}$, $f, g \in \mathcal{F}(M)$.
3. $1 = I$, where $1$ is the unity function constant on $M$, and $I$ is the identity operator on $\mathcal{H}$.
4. $\hat{q}_k, \hat{p}_k, k = 1, ..., n$ act irreducibly on $\mathcal{H}$.

The first condition requires to have an associated quantum operator for each observable.

The second condition may be taken as the consequence of the time-independence of the map $\hat{\cdot}$ for a wide class of dynamical systems on $(M, \omega)$, and is directly related to the dynamical problem of quantization. In particular, if the observable $f \in \mathcal{F}(M)$ has a complete Hamiltonian field (the integral curves $c_t$ through $c_0 = m$ given by $\dot{c}_t = X_f(c_t)$ are defined for $\forall t \in (-\infty, \infty)$, $\forall m \in M$), then the associated operator $\hat{f}$ must be self-adjoint, and generates a one-parameter group of unitary transformations on $\mathcal{H}$, $U_t^{(f)} = \exp(-\frac{i}{\hbar}\hat{f}t)$.

If the map $g \rightarrow \hat{g}$, $g \in \mathcal{F}(M)$ is time-independent, then $(\hat{g})_t = \hat{\cdot}(g_t)$, where $g_t = F_t^*g = g \cdot F_t$, ($F_t$ is the flow of $X_f$, $c_t = F_t(m)$), and $(\hat{g})_t = U_t^{(f)}(\hat{g}(U_t^{(f)})^{-1}$.

Locally, the equation $\hat{\cdot}(g \cdot F_t) = U_t^{(f)}(\hat{g}(U_t^{(f)})^{-1}$ becomes $\hat{\cdot}(L_{X_f}g) = -\frac{i}{\hbar}[\hat{f}, \hat{g}]$,

or $\hat{\{f, g\}} = -\frac{i}{\hbar}[\hat{f}, \hat{g}]$.

The third condition is imposed by the construction of the observables, accounting for the uncertainty relations of Heisenberg, or for the empiric wave-particle duality. Among the observables there are also constants which
are not naturally associated to the phase-space geometry, as the interaction strengths, the electric charge, or the mass. These act multiplicatively on the state vectors, as any real constants, behaving as multiples of the identity operator on $\mathcal{H}$. The third condition requires to quantize all the constants in the same way, irrespective if these are coming from the Poisson bracket of some observables (as the canonically conjugate coordinates), or if they represent dynamical constants of the classical system. In particular, the Heisenberg uncertainty relations are a consequence of this condition, proving its sufficiency.

The fourth condition accounts for the requirement of expressing the action of every operator associated to an observable through the action of the operators $\hat{q}^k, \hat{p}_k$, $k = 1, ..., n$. This requirement corresponds to the classical condition of expressing every observable as a function of the particular observables represented by the canonical coordinates $(q^k, p_k)$, $k = 1, ..., n$ on the phase space. Showing that every irreducible representation of the algebra $C_0 \equiv (q^1, q^2, ..., q^n, p_1, p_2, ..., p_n, 1)$ is unitarily equivalent to the Schrödinger representation, where $\mathcal{H} = L^2(R^n)$, $\hat{q}^k = q^k, \hat{p}_k = -i\hbar \frac{\partial}{\partial q^k}$, the Stone - von Neumann theorem (1932) [4] has given explicitly the space $\mathcal{H}$ and the map $f \rightarrow \hat{f}$.

In 1951 van Hove has proved rigorously the incompatibility between the four conditions stated above, proving therefore the impossibility of a complete quantization [4]. Moreover, he has shown that it is possible to fulfill the first three conditions, obtaining a ”prequantization”, but then the algebra $C_0$ is represented with infinite multiplicity. Also, if only the last three conditions are imposed, then the application $^\wedge$ must be restricted to some subalgebra $C \subset \mathcal{F}(M)$, containing $C_0$. In particular, the polynomial Hamiltonians quantizable within the Schrödinger representation are at most of second degree in coordinates and momenta.

These results have shown that the problem of the algebraic quantization has no meaning for the set of all observables contained in $\mathcal{F}(M)$, but only for a couple of subalgebras, $(C_0(M), C(M))$, $C_0(M) \subset C(M) \subset \mathcal{F}(M)$, with $C_0$ represented irreducibly.

For the manifolds $(M, \omega)$ which are not diffeomorphic to $(T^*R^n, \omega_0)$, (the de Rahm cohomology class $[\omega]_{dR} \neq 0$), the canonical coordinates $(q^k, p_k)$, $k = 1, 2, ..., n$ are only locally defined and are not observables, so that the fourth condition must be reformulated. A direct generalization concerns the
homogeneous symplectic spaces \((M, \omega)\) onto which a Lie group \(G\) acts transitively and strongly symplectic. The action of \(G\) is defined globally by a homomorphism \(\sigma : G \to \text{Ham}(M)\) and locally by the map \(d\sigma : g \to \text{ham}(M)\). Here \(\text{Ham}(M)\) is the group of Hamiltonian diffeomorphisms of \(M\), \(g\) denotes the Lie algebra of \(G\), and \(\text{ham}(M)\) is the Lie algebra of Hamiltonian fields on \(M\). A lift of the map \(d\sigma\) is a Lie algebra homomorphism \(\lambda : g \to \mathcal{F}(M)\) [5] such that the following diagram is commutative.

\[
\begin{array}{cccc}
0 & \to & R & \to & \mathcal{F}(M) & \to & \text{ham}(M) & \to & 0 \\
\uparrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
\lambda & \uparrow & & & & d\sigma & \downarrow & & & \uparrow & \\
g & & & & & & \lambda(g) & & & \lambda(g) & \\
\end{array}
\]

This lift exists iff the 2-cocycle \(\mu : g \times g \to R\),

\[
\mu(x, y) = \{\mu_0(x), \mu_0(y)\} - \mu_0([x, y]) , \quad x, y \in g
\]

(with \(\mu_0 : g \to \mathcal{F}(M)\) any linear map making the diagram to commute), has a vanishing de Rahm class \([\mu]_{dR} \in H^2(g, R)\) [5] [6]. Using the map \(\lambda\), the fourth condition defining the Hilbert space can be formulated as:

4'. If \((M, \omega)\) is a strong symplectic homogeneous \(G\)-space, and \(\lambda\) is a lift of the map \(d\sigma\), then the subalgebra \(\mathcal{C}\) of the quantizable observables must contain the subspace \(\lambda(g)\), and the representation Hilbert space \(\mathcal{H}\) must be irreducible with respect to the action of the operators from \(\hat{(\lambda(g))}\) [7].

As a first step towards quantization, the prequantization of the algebra \(\mathcal{F}(M)\) was obtained geometrically [6] - [8] by constructing a Hilbert space \(\mathcal{H}_M\) as a space \(\Gamma_L\) of sections in a hermitian line bundle with connection \((L, \alpha)\) over \((M, \omega)\). Requiring the symplectic form \(\omega\) to be the curvature of the connection [6] \((d\pi^*\alpha = \omega, \text{with } \pi : L \to M \text{ the projection on the base in } L)\), the line bundle exists only in special cases, namely when \(\omega\) fulfills the Weil's integrality condition: \(h^{-1}[\omega]_{dR} \in Z\). This condition acts similarly to the BWS condition of the old quantum mechanics, selecting the classical manifolds of observables compatible with the description of a quantum system. In particular, for the integrable systems the Weil condition for the reduced phase space and BWS quantization rule become the same.

In the case \(M = T^*R^n\) the prequantum Hilbert space \(\mathcal{H}_M\) is represented by:

\[
\mathcal{L}^2(R^{2n}) = \{\Psi : M \to C, \int |\Psi|^2 |\omega^n| < \infty\}
\]
where $|\omega^n|$ is the natural volume on $R^{2n}$. Because this space is too large for quantization, it was investigated the possibility to extract a "quantum subspace" $H_P \subset H_M$ generated by the sections from $\Gamma_L$ which are constant on the leaves of an integrable foliation of $M$ by Lagrangean submanifolds (a polarization $P$ on $M$). The subspace $H_P$ is not invariant to the action of all the operators associated with observables, and consequently the subalgebra of the observables quantizable within $H_P$ is $C_P = \{ f \in \mathcal{F}(M), f H_P \subset H_P \}$. 

This procedure of quantization has the advantage of giving a natural correspondence between the spaces $H_P$ and $H_{P'}$ associated to different polarizations $P$ and $P'$, as subspaces of the whole prequantum space $H_M$. Unfortunately, it cannot be physically accepted because in many important cases, including the Schrödinger quantization of $T^*R^n$, $H_P$ does not exist.

An alternative solution is to construct an intrinsic Hilbert space $H^{[\mu]}_P$ associated to the polarization $P$ independently of the prequantum space $H_M$. With some enough general restrictions, the space $H^{[\mu]}_P$ corresponds to a class of measures $[\mu]$, Lebesgue equivalent, defined on a Lagrangean submanifold $Q \subset M$, transversal to $P$, whose elements are called half-densities. This formalism has solved the problem of quantization for a wide class of physically relevant Hamiltonians, but the results are still slightly different from those obtained by using the standard quantum mechanics, well supported by experiments. Thus, the energy $\epsilon_n = n\hbar\nu, n = 0, 1, 2, \ldots$ predicted for the one-dimensional harmonic oscillator is different from the correct result $\epsilon_n = (n + 1/2)\hbar\nu$ [7]. Such differences were further eliminated by assigning a metalinear structure to the Lagrangean submanifold $Q$, and correspondingly extending the half-densities Hilbert space $H^{[\mu]}_P$ to a Hilbert space of half-forms $H^{A,1/2}_P$ [7]. As a rule, its construction is cumbersome, and the half-forms quantization was tested only for a small number of simple systems.
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