Quantization of mechanical systems

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Abstract

In this paper we show what seems to be the (very simple) key for quantization of classical systems. Given a manifold $M$, each pair given by a riemannian metric (nondegenerate, of arbitrary signature) and a linear connection, canonically determine a quantization rule or ‘Correspondence Principle’, which assigns to each classical magnitude (function in $TM$, subject to certain conditions) a differential operator in $C^\infty(M)$. The issue about the order in which the $p'$ and $q'$ are to be taken in quantization loses all meaning, when the general rule has been fixed. Once specified the Correspondence Principle, each ‘classical state’ of the system, understood as a vector field on $M$, determines a wave equation for each magnitude. The Schrödinger equation is a particular example of these wave equations.

1. Introduction

The problem of quantization of classical mechanical systems has been dealt with in thousands of works [1]. Even for configuration spaces with flat metric, the problem seems strongly non-trivial [2].

Most physicists consider Classical Mechanics merely as a limiting case of Quantum Mechanics (when $\hbar \to 0$ or masses $\to \infty$). From this point of view, the problem of quantization of classical systems consists of guess the right quantum equations, which give the classical ones in the limit. The essential problems are to find the general formalism for Quantum Mechanics and its interpretation. For this reason, from the texts of Von Neumann and Dirac to the present ones, the problem of the quantization of classical systems has usually been reduced to establishing the rules of commutation of the $p$ and $q$ and to notice that, in each case, one has to guess the good order in which are written for the Hamiltonian and the momenta (for a quite recent text where the problem of quantization is taken in consideration, see [3, chapter XIII]).

Many other physicists and mathematicians have sought bridges that link Classical to Quantum Mechanics. The problem has always appeared as remarkably complex. We have found one canonical and simple bridge. It is a method of quantization valid for any classical mechanical system, it is canonically constructed and, in the case of flat configuration space, gives the usual quantization rules.

The hamiltonian formalism of the Classical Mechanics is expressed in terms of the symplectic structure of the phase space $T^\ast M (M = \text{ configuration space})$. The theory of first order partial differential equations, due to Jacobi [4], was developed by Lie [5, 6] in the language of the symplectic manifolds. The set $C^\infty(T^\ast M)$ is endowed with the structure of algebra by means of the Poisson bracket. The maximal commutative subalgebras (algebras of functions in involution) give the (local) lagrangian fibrations of $T^\ast M$, which are the complete integrals of the partial differential equations defined by each function of that subalgebra. The analogies: Poisson bracket—Commutator of operators, Maximal subalgebra of functions in involution—Complete system of commuting observables, Lagrangian manifold—Pure quantum state, suggest that the key of the quantization can be found in the symplectic structure, without further data. But attempts in that direction have failed.

In fact, the symplectic structure of the phase space leaves out essential data of the mechanical system, which are associated with $TM$, not directly to $T^\ast M$. As an example, it is unknown how to decide when a tangent vector field on $T^\ast M$ is a second order differential equation if an isomorphism $TM \approx T^\ast M$ (by means of a metric on $M$) has not previously been established. For the same reason, the ‘time’ on $T^\ast M$ can only be considered as an external
parameter because it is an structure essentially linked to the notion of second order differential equation, so to \( TM \) [7, 8].

In the present work, we propose a rule of quantization for classical mechanical systems on an arbitrary configuration space \( M \) (finite dimensional smooth manifold), which starts from the duality \((TM, T^*M)\) and depends on two data: a riemannian metric \( T_2 \) (of arbitrary signature) on \( M \) and a linear connection \( \nabla \) on \( TM; \nabla \) can be the Levi-Civita connection associated with the metric \( T_2 \), which produces a quantization canonically associated with \((M, T_2)\), that, in the case \( M = \mathbb{R}^n, T_2 = \) flat metric (arbitrary signature), coincides with the 'canonical quantization' established by Dirac in cartesian coordinates. However, each \( \nabla \) determines a quantization rule (once fixed \( T_2 \)). The simplicity and generality of our method is build on the idea of copy each function in the configuration space \( M \) to a function on each fibre of \( TM \) by means of the riemannian exponential map. For another interesting approach to invariant quantization, see [9].

The quantized magnitudes, in the general case, are the complex valued functions on \( TM \) that are polynomials along the fibres. Such functions are that associated with symmetric covariant tensors (homogeneous or not, with complex values) on \( M \). We will call them classical magnitudes. Given the triplet \((M, T_2, \nabla)\), each covariant symmetric tensor \( a \) on \( M \), determines a classical magnitude \( a \in C^\infty(TM) \) and a differential operator \( \hat{a} \) on \( C^\infty(M) \). The correspondence \( a \mapsto \hat{a} \) is the rule of quantization.

The possibility of extending that correspondence to functions more general than the classical magnitudes depends on the data \((M, T_2, \nabla)\). As an example, for \( M = \mathbb{R}^n \) and flat \( T_2 \), such an extension can be carried out (not univocally) to the fields assigning with each \( x \in M \) an arbitrary distribution on \( T_xM; \) the operator \( \hat{a} \) corresponding with such a field \( a \) will not be, in general, a differential operator. But this problem of extension of the quantization rule to general functions or distributions is not the subject of the present work.

Assuming that \( M \) is oriented, metric \( T_2 \) gives a volume form, that allows one to integrate functions and, with it, to define the Hilbert space \( L^2(M) \). Which of the operators \( \hat{a} \) will be self-adjoint or normal depends on the data \( T_2, \nabla \). Anyway, there is an essential fact: for any \( T_2 \), if \( \nabla \) is the associated Levi-Civita connection, the differential operator that quantizes the kinetic energy function \( T(\cdot) \), that is, the function associated with \((1/2)T_2\), understanding that the masses are included into \( T_2 \), is \(-\frac{\hbar^2}{2}\Delta\), where \( \Delta \) is the laplacian operator of the given metric. Besides, \( \Delta \) is always self-adjoint on \( L^2(M) \). Therefore, for each conservative system with hamiltonian \( H = T + U \), the hamiltonian operator \( \hat{H} \) is self-adjoint, and the Schrödinger equation for the time evolution of that system gives a law described by the action of an 1-parametric group of unitary automorphisms acting on \( L^2(M) \). The problem here is the meaning of ‘time’ in Quantum Mechanics; classical time is defined by the trajectories of the second order differential equations, but in Quantum Mechanics the notion of trajectory ceases of make sense.

We will not deal in this work with the problem of time and the temporal evolution in Quantum Mechanics. For these questions, see preprint [8].

The analogy Poisson bracket—Commutator of operators, has guided the quantization process from the beginning [10]. Of course, the general formula \([\hat{a}, \hat{b}] = -i\hbar [a, b]\) can not be fulfilled in any quantization process. But, whatever the quantization process, the two members of the equation as differential operators have, in general, the same symbol. That coincidence, can be vaguely understood as a coincidence of the commutator of operators with the Poisson bracket, in the limit of the big momenta or large distances. But neither is this the main topic of our work.

The quantization process we propose is not limited to \((M, T_2)\) interpreted as the configuration space of a classical mechanical system. For instance, the tensors appearing in the Einstein field equations are covariant symmetric tensors. Therefore, they are classical magnitudes and, so, quantizable.

### 2. Physical magnitudes

Let \( M \) be a smooth manifold of dimension \( n \), \( TM \) be its tangent bundle and \( T^*M \) be its cotangent bundle; let \( C^\infty(M) \) denote the ring of complex valued (infinitely) differentiable functions in \( M \).

On \( T^*M \) we define the Liouville form \( \theta \), by \( \theta_p = \alpha, \) for each \( \alpha \in T^*M \). In what equality it is understood that \( \alpha \) is lifted by pull-back from \( M \) to \( T^*M \). In local coordinates \((x^1, \ldots, x^n)\) for \( M \) and the corresponding ones \((x^1, \ldots, x^n, p_1, \ldots, p_n)\) for \( T^*M \), the expression of the Liouville form is \( \theta = p_i \, dx^i \) (summation with respect repeated indexes is assumed). The 2-form \( \omega_2 = d\theta \) is the symplectic form in \( T^*M \); its expression in local coordinates is \( \omega_2 = dp_i \wedge dx^i \).

The interior product with \( \omega_2 \) establishes an isomorphism of \( C^\infty(T^*M) \)-modules between tangent vector fields on \( T^*M \) and differential 1-forms on \( T^*M \): \( D \mapsto D_{\omega_2} \). In this isomorphism, the vertical tangent fields (those that, as derivations, annihilate the subring \( C^\infty(M) \) of \( C^\infty(T^*M) \)) correspond to the horizontal 1-forms (those 1-forms annihilated, by interior product, by vertical fields).

In local coordinates, the vertical tangent field \( \partial / \partial \theta \) is applied on \( dx^i \).
The isomorphism established by the symplectic form between the \( C^\infty(T^*M) \)-modules of vertical fields and horizontal 1-forms, is naturally extended to an isomorphism between the tensor algebra of the ‘vertical’ contravariant tensor and the ‘horizontal’ covariant tensor algebras.

For our present purpose we are not interested in all these tensors, but only those corresponding to symmetrical covariant tensors on \( M \): let \( \mathcal{A} \) be the \( C^\infty(M) \)-algebra of symmetric covariant tensors on \( M \), considered (after pull-back) as covariant tensors on \( T^*M \); the symplectic form made to \( \mathcal{A} \) a \( C^\infty(M) \)-algebra \( \mathcal{A}^\ast \) of symmetric contravariant tensor fields on \( T^*M \). In local coordinates, the polynomial \( P(\partial/\partial p_1, \ldots, \partial/\partial p_n) \) with coefficients in \( C^\infty(M) \), corresponds to the polynomial with the same coefficients, \( P(\partial/\partial p_1, \ldots, \partial/\partial p_n) \in \mathcal{A}^\ast \).

In the tangent bundle the notions of vertical tangent field and horizontal 1-forms are analogous to those we just have considered in \( T^*M \). In local coordinates \((x^1, \ldots, x^n, \dot{x}^1, \ldots, \dot{x}^n)\), the horizontal 1-forms are the linear combinations of the \( dx^i \) with coefficients in \( C^\infty(TM) \) and vertical tangent fields are linear combinations of the \( \partial/\partial x^i \). But here, if no additional structure to that of manifold is given, we have no symplectic form.

The realization of the tensor algebra \( \mathcal{A} \) that, in \( T^*M \), was given as an algebra of vertical differential operators, in \( TM \) is given as an algebra of functions as follows: for each function \( f \in C^\infty(M) \) let us denote by \( \hat{f} \) the function on \( T^*M \) defined by the rule \( \hat{f}(v) = f(\hat{v}) \), for each \( v \in TM \) considered as a derivation \( v: C^\infty(M) \rightarrow \mathbb{R} \); the function \( \hat{f} \) is, essentially, \( df \). In general, for each horizontal 1-form \( \alpha \) on \( TM \) it is defined the function \( \hat{\alpha} \) by \( \hat{\alpha}(v) = \langle \alpha, v \rangle \) (duality). By means of this rule, each tensor \( a \in \mathcal{A} \) define a function \( \hat{a} \in C^\infty(TM) \), that is polynomial in the fibres (a polynomial in the \( \dot{x}^i \) with coefficients in \( C^\infty(M) \)). The function \( \hat{a} \) is, essentially, the same thing as the tensor \( a \).

In conservative mechanical systems, which are now our main subject of interest, all the magnitudes appearing in the space of position-velocity states are of this type. For that reason, these functions \( g \) will be called classical magnitudes; the ring of the classical magnitudes is, then, the ring \( \mathcal{A} \cong \mathcal{A}^\ast \) obtained by associating to each tensor \( a \in \mathcal{A} \) the function \( \hat{a} \). In local coordinates, \( \hat{a}(x^1, \ldots, x^n) \) is obtained if \( dx^i \) is replaced by \( \dot{x}^i \) in the polynomial \( a(dx^1, \ldots, dx^n) \). As \( C^\infty(M) \)-algebras we have isomorphisms:

\[
\mathcal{A} \cong \mathcal{A} \cong \mathcal{A}^\ast,
\]

in such a way that each classical magnitude \( g \) (function on \( TM \)) is, substantially, the same object as (canonically identified to) the corresponding vertical differential operator on \( T^*M \).

It is convenient to establish this correspondence on a different way, by using the Fourier transform, as follows:

The Liouville form can be interpreted as a function on the fibre product \( TM \times_M T^*M \), by assigning to each vector \( v_x \in T_xM \) and each 1-form \( \alpha_x \in T^*_xM \) the value

\[
\theta(v_x, \alpha_x) = \langle v_x, \alpha_x \rangle.
\]

When ‘dimensions’ are introduced for the classical magnitudes, \( \theta \) has the dimension of ‘action’. For this reason, in order to give full sense to the transcendent functions of \( \theta \) and they have a meaning independent of the units of measure, a constant \( \hbar \) must be introduced with the dimensions of ‘action’ taking \( \theta/\hbar \) instead of \( \theta \). With this in mind, the function \( \exp(i\theta/\hbar) \) on \( TM \times_M T^*M \) makes sense.

To be specific, let us take as base space for the Fourier transform \( S(TM) \), the set of complex valued functions defined on \( TM \), that on each fibre \( T_xM \) are \( C^\infty \) and rapidly decreasing they and all their derivatives. Analogous meaning for \( S(T^*M) \).

In each fibre \( T_xM \cong \mathbb{R}^n \), the usual measure is, up to a constant factor, the unique translation invariant (Haar measure of the group \( \mathbb{R}^n \)). Once this Haar measure is chosen on each fibre, we can define the Fourier transform fibre to fibre:

\[
\mathcal{F}: S(TM) \rightarrow S(T^*M), \quad f \mapsto \mathcal{F}f,
\]

where

\[
(\mathcal{F}f)(\alpha_x) = \int_{T_xM} f(v_x) e^{i\theta(v_x, \alpha_x)} d\mu(v_x),
\]

being \( d\mu \) the Haar measure fixed on \( T_xM \).

By taking local coordinates \((x^1, \ldots, x^n)\) on an open set \( U \) of \( M \) and the corresponding ones \((x^1, \ldots, x^n, \dot{x}^1, \ldots, \dot{x}^n)\) on \( TU, (x^1, \ldots, x^n, p_1, \ldots, p_n) \) in \( T^*U \), we have \( \theta(x, p) = p \dot{x} \) and then:

\[
(\mathcal{F}f)(x, p) = \lambda_x \int_{T_xM} f(x, \dot{x}) e^{i\theta/\hbar} dx^1 \cdots dx^n,
\]

where \( \lambda_x \) is the constant that fixes the choice of the measure.

By derivation under the integral sign the classical formula is obtained:

\[
\mathcal{F}(\hat{g})(x, \dot{x}) = g(x, -i\hbar \partial/\partial p)(\mathcal{F}f)(x, p)
\]

for any function \( g \) on \( TM \) that is polynomial in the \( \dot{x} \), that is to say, for each symmetric covariant tensor \( a \) on \( M \).
We see that, by changing the symplectic form $\omega_2$ by $(i/\hbar)\omega_2$, the correspondence between classical magnitudes $\varrho \in \mathcal{A}$ and vertical differential operators on $TM$ is the same as the one given by the Fourier transform. By introducing now the factor $i/\hbar$, we will denote by $A$ the vertical differential operator on $TM$ that corresponds to the magnitude $\varrho$:

$$\varrho(x, \dot{x}) \leftrightarrow a(x, dx) \leftrightarrow A(x, \partial/\partial p) = \varrho(x, -i\hbar \partial/\partial p).$$

$\varrho$ and $A$ are the expressions on $TM, T^*M$ of the same object, the tensor $a$. In local coordinates, the correspondence is

$$a_{j_1, \ldots, j_n}(x) \dot{x}^{j_1} \cdots \dot{x}^{j_n} \leftrightarrow a_{j_1, \ldots, j_n}(x) dx^{j_1} \cdots dx^{j_n} \leftrightarrow a_{j_1, \ldots, j_n}(x) (-i\hbar)^n \frac{\partial^n}{\partial p_{j_1} \cdots \partial p_{j_n}},$$

where the $a_{j_1, \ldots, j_n} \in C^\infty(M)$ denote the coefficients of the tensor $a$.

### 3. Introducing a metric on M Quantization

When the structure of smooth manifold is the only one given on $M$, there is no correspondence between points of $TM$ and points of $T^*M$, although the symplectic structure (or the Fourier transform fiberwise) has allowed us to establish the correspondence $\varrho \rightarrow A$ between functions on $TM$ which are polynomial on fibres and vertical differential operators on $T^*M$.

Let $T_2$ be a riemannian metric (of arbitrary signature) given on $M$. The metric establishes an isomorphism of fibre bundles $TM \rightarrow T^*_M$ by assigning to each tangent vector $v_\mu \in T_xM$ the differential 1-form $\alpha_\mu = v_\mu \circ T_2 \in T^*_xM$ (inner product of $v_\mu$ with $T_2$). By means of that isomorphism we can translate each structure from one to the other of those bundles; we can talk about the Liouville form, the symplectic form, etc, on $TM$. In order to simplify the notation, if there is no risk of confusion, we will use the same notation for each object on $TM$ and its translation to $T^*M$. In this way, if the local coordinated expression for the metric is

$$T_2 = g_\mu dx^\mu dx^\nu,$$

the function $p_\mu$ on $T^*M$ is, in the coordinates of $TM, p_\mu = g^\mu_\nu \dot{x}^\nu$, and

$$\frac{\partial}{\partial p_\mu} = g^\mu_\nu \frac{\partial}{\partial x^\nu}.$$

In the previously established correspondence $\varrho \rightarrow A$, to the function $x^\mu$ there corresponds $-i\hbar \partial/\partial p_\mu$; therefore, to the polynomial $p_\mu = g^\mu_\nu \dot{x}^\nu$ it corresponds

$$-i\hbar g^\mu_\nu \frac{\partial}{\partial p_\mu} = -i\hbar g^\mu_\nu \frac{\partial}{\partial x^\nu} = -i\hbar \frac{\partial}{\partial \dot{x}^\nu}.$$

To the very metric tensor $T_2$ there corresponds on $TM$ the function $2T = g^\mu_\nu \dot{x}^\nu \dot{x}^\mu$ and, on $T^*M$, the differential operator $\Delta = -\hbar^2 g^\mu_\nu \partial/\partial p_\mu \partial/\partial p_\nu$, which, once introduced the metric on $M$ becomes

$$\Delta = -\hbar^2 g^\mu_\nu g^\nu_\sigma \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\sigma} = -\hbar^2 g^\mu_\nu \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\nu}.$$

Now, let $\nabla$ be a linear connection on $M$ (for instance, the Levi-Civita connection associated with the metric $T_2$). For each point $x_0 \in M$ the connection $\nabla$ establishes a local isomorphism between a certain neighbourhood $U$ of the origin in $T_{x_0}M$ and a neighbourhood $\mathcal{V}$ of $x_0$ in $M$:

$$\exp: \mathcal{V} \rightarrow U$$

which sends each vector $v_{x_0} \in T_{x_0}M$ to the point $\exp(v_{x_0})$ which is the end point of the arc of geodesic path in $M$ parametrized by $[0,1]$ and starting at $x_0$ with tangent vector $v_{x_0}$.

By taking local coordinates $(x^\mu)$ on an neighbourhood of $x_0$ in $M$ and the corresponding ones $(\dot{x}^\mu, \ddot{x}^\mu)$ in $TM$, the expression of $\exp$ is

$$\dot{x}^\mu = x^\mu_0 + \dot{x}^\mu - \frac{1}{2} \Gamma^\mu_{\nu \sigma}(x_0) \dot{x}^\nu \ddot{x}^\sigma + \cdots,$$

(3.1)

(where the $\Gamma^\mu_{\nu \sigma}$ are the Christoffel symbols of the connection $\nabla$), if we get the Taylor expansion till second order terms. That formula is easily derived from the differential equation defining the geodesics and, from it and the inverse function theorem it results that $\exp$ is a local differentiable isomorphism. For further details, see [11].

The exponential map allows us to assign to each function $f \in C^\infty(M)$ a function $\hat{f}$, defined on a neighbourhood of the 0 section of $TM$, by means of the rule $\hat{f}(v_\mu) = f(\exp(v_\mu))$ for the $v_\mu \in T_{x_0}M$ on which the exponential map is defined. The function $\hat{f}$ is the description of $f$ done from each point of the configuration space (from ‘each observer’). If we denote by $\mathcal{O}(M)$ the ring of germs of $C^\infty$ functions on neighbourhoods of 0
section of $TM$, the assignation $f \rightarrow \tilde{f}$ determines an injection of $C^\infty(M)$ into $\mathcal{O}(M)$ that we will call the riemannian injection.

The trivial injection $C^\infty(M) \rightarrow C^\infty(TM)$ given by the pull-back associated with the projection $TM \rightarrow M$, translates all vertical differential operators in $TM$ without 0-order terms, to the identically 0 operator in $C^\infty(M)$. But, thanks to the riemannian immersion, each differential operator $A$ in $TM$ gives on $M$ a non trivial differential operator:

$$\hat{a} f := (A \tilde{f})|_0 \text{ section},$$

by identifying $M$ with the 0-section of $TM$.

And this seems to be the key of the quantization:

**Definition 3.1.** Let $a$ be a symmetric covariant tensor on $M$, $g \in C^\infty(TM)$ its associated function (‘classical magnitude’) and $A$ the vertical differential operator in $TM$ corresponding to $a$ (once identified $TM$ and $T^*M$ by means of the metric). The differential operator

$$\hat{a} \colon C^\infty(M) \rightarrow C^\infty(M)$$

derived from $A$ by means of the riemannian injection $C^\infty(M) \rightarrow \mathcal{O}(M)$ is the quantization of the magnitude $a$.

The quantization $g \rightarrow \hat{a}$ is $C^\infty(M)$-linear for the module structure in the set of differential operators (given by the left multiplication by functions). The quantization is also injective, since, if the vertical differential operator $A$ annihilates all $\tilde{f}$ coming from $C^\infty(M)$, it holds $A = 0$. That is because on each fibre of $TM$, $A$ is a polynomial in the $\partial/\partial x$ with constant coefficients. However, the multiplicative structure changes, so losing the commutativity. Given two symmetric covariant tensors $a, b$ in $M$, for each $f \in C^\infty(M)$, the computation of $\partial b(\hat{a} f)$ is made by applying the differential operator $B$ to the function $\hat{a} f$, that differs from $A \tilde{f}$; this is why, in general, it does not hold $\partial b \circ \hat{a} = \hat{b}a$. In general neither is true $\hat{a}^2 = \hat{a}^2$, as we will see later in some particular instance.

For the time being, the Taylor expansion of second order of the exponential map, allows us to find the quantum operators corresponding to the functions that are polynomials of degree lower or equal than 2 in the $\dot{x}$.

For each $f \in C^\infty(M)$ we have

$$\left(\frac{\partial \tilde{f}}{\partial x^i}\right)(0) = \left(\frac{\partial f}{\partial x^i}\right)(x_0), \quad \text{and hence,} \quad \hat{b}_j = -ih \frac{\partial}{\partial x^j}.$$ 

It follows that for each 1-form $\alpha$ on $M$, we have

$$\hat{\alpha} = -ih \text{ grad } \alpha.$$ 

For example, in $\mathbb{R}^3$ with Euclidean coordinates $x, y, z$ and metric $T_2 = m(dx^2 + dy^2 + dz^2)$, (where $m$ denotes the mass of a particle), to the form $\alpha = m(xdy - ydx)$ it corresponds the classical function $f = m(x\dot{y} - y\dot{x})$ and

$$\hat{\alpha} = -ih x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}.$$ 

For second order derivatives, when $\nabla$ is the Levi-Civita connection, an easy computation gives

$$\left(\frac{\partial^2 \tilde{f}}{\partial x^k \partial x^l}\right)(0) = \left(\frac{\partial^2 f}{\partial x^k \partial x^l} - \Gamma^j_{kl} \frac{\partial f}{\partial x^j}\right)(x_0).$$

As a consequence, for the very metric tensor $T_2$ we get

$$2 \hat{T} f = -h^2 g^{k\ell} \left(\frac{\partial^2 f}{\partial x^k \partial x^\ell} - \Gamma^j_{kl} \frac{\partial f}{\partial x^j}\right) = -h^2 \Delta f,$$

where $\Delta$ is the laplacian operator associated with the metric. Recall that the masses are considered as included in the coefficients $g_{kl}$ of $T_2$.

For the computation of $\hat{a}$ when $a$ has arbitrary order, the formulae in [11] can be used.

**Remark 3.1.** The quantization is a local operation in $M$.

**Remark 3.2.** The correspondence $g \rightarrow \hat{a}$ is established for the tensor as a whole and it cannot be ‘factorized’ because, in the general case, is not even $\hat{a}^2 = \hat{a}^2$. 


Remark 3.3. It is generally false that the Poisson bracket \( \{ a, b \} \) corresponds to the commutator \([\hat{a}, \hat{b}]\): in fact \( \{ a, b \} \) contains just first order derivatives of the coefficients of tensors \( a, b \), while in \([\hat{a}, \hat{b}]\) appear, in general, derivatives whose order is the greatest order of \( a, b \). A simple calculus gives

\[
[\hat{a}, \hat{b}] = -i\hbar \begin{pmatrix} [\hat{a}, \hat{b}] + (\text{operators of order} \leq o(a) + o(b) - 2),
\end{pmatrix}
\]

where \( o(a) \) and \( o(b) \) indicate the respective orders. In the general case, \([\hat{a}, \hat{b}]\) and \([\hat{a}, \hat{b}]\) are both of order \( o(a) + o(b) - 1 \). When this occurs, \([\hat{a}, \hat{b}]\) and \(-i\hbar \begin{pmatrix} a, b \end{pmatrix}\) acting on \( \exp(i\lambda p \cdot x) \), asymptotically coincide for \( \lambda \to \infty \).

4. Wave equations. Schrödinger equation

The classical magnitudes \( a \) that we are considering, are functions in \( TM \), which are not automatically operators on \( C^\infty(M) \) (except when \( a \) is a tensor of order 0, a function in \( M \)).

For each section \( u: M \to TM \) (a vector field on \( M \)), the restriction \( \hat{a}(u) \) of the function \( a \) to the section \( u \), is transported as a function on \( M \) and, as such, operates by multiplication on \( C^\infty(M) \).

Functions \( \Psi \) in \( C^\infty(M) \), or in a prefixed space of functions or distributions, where operators \( \hat{a} \) and \( \hat{a}(u) \) coincide are the proper functions for the magnitude \( a \) in the classical state \( u \). They are the solutions of the wave equations

\[
(\hat{a} - \hat{a}(u))\Psi = 0.
\]

When the tensor \( a \) is a function in \( C^\infty(M) \), we have \( \hat{a} = a = \hat{a} \) and the wave equation is trivial. This fact does not prevent us to consider wave equations that are not associated with sections \( u \); for instance, the equation for the position operator \( \hat{x}\psi = \lambda \psi \) on \( M = \mathbb{R} \), which has as solutions the Dirac \( \delta \)'s. In general, for any classical magnitude \( a \), it can be considered the equation of the ‘eigenfunctions’ of \( \hat{a}: \hat{a}\psi = \lambda \psi \), in the space of admissible functions or distributions \( \Psi \). For each eigenvalue \( \lambda \), the equation \( \hat{a} = \lambda \) determines a submanifold of \( TM \); in the previous example, \( a = x \), the submanifold \( x = \lambda \) is a fibre of \( TR \to \mathbb{R} \) (arbitrary \( x \)). More generally, if tensor \( a \) is real and \( \lambda \) is a real eigenvalue of \( \hat{a} \), the first order partial differential equation \( \hat{a} = \lambda \) can admit as non classical solution a Lagrangian manifold which is not a section of \( TM \rightarrow M \).

The most important example of wave equation is the Schrödinger equation. When \( \nabla \) is the Levi-Civita connection, for a conservative mechanical system with Hamiltonian \( H = T + U \), the quantization of \( H \) is

\[
\hat{H} = -\frac{1}{2} \hbar^2 \Delta + U
\]

and the wave equation is

\[
\left( -\frac{1}{2} \hbar^2 \Delta + U \right) \Psi = H(u)\Psi.
\]

When \( u \) is a section (a classical state of the system at each point of \( M \)) of constant energy \( E \), the previous equation becomes the Schrödinger equation. In particular, when \( u \) is a Lagrangian section, \( u = \text{grad } S \), the equation \( H(u) = E \) is the Hamilton–Jacobi equation for the ‘action’ \( S \). This equation has solutions for all the values taken for the function \( H \) in the space of states. The Schrödinger equation impose on the values of the energy \( E \) the condition of admitting non trivial solutions \( \Psi \): it selects a subset of values admissible for the energy \( H \).

5. Klein–Gordon equation

As another example, let us consider a mechanical system defined by the Lorentz force. Let \( (M, T_2) \) be as above and let \( F_2 \) be an electromagnetic field: a closed differential two form on \( M \), \( dF_2 = 0 \). Assume that \( F_2 \) admits a vector potential \( A \) (which is always locally true), that is to say, \( F_2 = dA^a \), where \( A^a = A_{\ldots 2} \). It can be seen \[12,13\] that the corresponding Newton equation can be written in the following way:

\[
D_\mu (d\theta^\mu + F_2) + dT = 0,
\]

where \( D = \hat{\theta}^j / \partial x^j + \hat{\psi} / \partial \psi \) is the second order differential equation whose trajectories describe the evolution of this mechanical system. That equation takes the form of Hamiltonian equations if replace the 2-form \( \omega_2 = d\theta = dp^i \wedge dx^i \) by \( \omega_2 = d\theta + F_2 = d(\theta + A^a) = d(p^i + A_i) \wedge dx^i \) (‘minimal coupling’). In this way, \((TM, \omega_2)\) (or \((TM, \omega_2)\)) if we use the identification produced by \( F_2 \) defines a symplectic structure and the previous Newton equation can be written as

\[
D_\mu \omega_2 + dT = 0. \tag{5.1}
\]
In other words, $D$ is the hamiltonian vector field associated with the kinetic energy function $T$ (in the symplectic manifold $(TM, \omega_B)$).

In this context we proceed to define the Hamilton–Jacobi equation as it was done for conservative systems (see [12, 13]). An intermediate integral $u$ of the second order differential equation $D$ is, by definition, a tangent vector field $u: M \rightarrow TM$ (a first order differential equation) whose solutions are also solutions of $D$. When the symplectic form $\omega_B$ vanishes on the image of $u$ in $TM$ (or $T^*M$) we say that $u$ is $\omega_B$-Lagrangian (this is equivalent to be locally exact $u + A = \text{grad} S$ in $TM$ or $u \cup T_2 + A^* = dS$ in $T^*M$, respectively, for a suitable function $S \in C^\infty(M)$; also we can see that $-u$ is another vector potential for $F_2$). Then the Hamilton–Jacobi equation is the equation describing the Lagrangian intermediate integrals of (5.1). In this case, we have, for a constant $\mu$:

$$T(u) = \frac{1}{2} \| u \|^2 = T(\text{grad} S - A) = \mu,$$

or, which is the same,

$$\frac{1}{2} \| \text{grad} S \|^2 - A \cdot \text{grad} S + \frac{1}{2} \| A \|^2 = \mu.$$

This means that the classical magnitude $T - A^* + \frac{1}{2} \| A \|^2$ along the section grad $S: M \rightarrow TM$ is a constant $\mu$. This 'Hamilton–Jacobi' equation is quantized (if $\nabla$ is the Levi-Civita connection) as the Klein–Gordon equation:

$$\left[ -\frac{\hbar^2}{2} \Delta + i\hbar A + \frac{1}{2} \| A \|^2 \right] \Phi = \mu \Phi. \quad (5.2)$$

**Remark 5.1.** The problem of finding intermediate integrals $u$ which are simultaneously vector potentials for $F_2$ was considered by Dirac [14] in the Minkowski space $\mathbb{R}^4$. In that work, Dirac considers ad hoc the constraint $T(u) = \text{constant}$. In [15] was proved that if the current $u$ (that is to say, $u^a := \text{div} F_2$ as defined by the Maxwell equations) is a lagrangian intermediate integral of (5.1) (so that locally $u = -A + dS$ for a suitable function $S$, or equivalently, $-u$ is a vector potential and if $A$ is taken without divergence, then $T(u)$ is a constant and $\Phi := e^{\mu \Phi}$ is a solution of the Klein–Gordon equation (5.2). Thus, if we impose obedience to the Lorentz force on the current, quantum conditions result.

6. The problem of the time evolution

Our intuition of time is the newtonian one: time 'flows equably without relation to anything external' (Scholium to the definitions in the Principia). For this reason we can accept without too much criticism the introduction of time in Quantum Mechanics rewriting the Schrödinger equation in the form $\hat{H} \Phi = i\hbar \frac{\partial \Phi}{\partial t}$, with $\Phi = e^{-i\frac{\hat{H}}{\hbar} \tau}$; the so modified 'time dependent Schrödinger equation' admits as solutions the superposition of stationary states $e^{-i\frac{\hat{H}}{\hbar} \tau} \psi_0$, and the time evolution in the space of states is that of the one parametric group $\{ e^{-i\frac{\hat{H}}{\hbar} \tau} \}_{\tau \in \mathbb{R}}$.

When one takes as space of admissible 'pure' states for the quantum-mechanic system the Hilbert space (complex and separable), the Stone theorem about unitary one-parametric groups of automorphism (see [16]) allows us to invert the direction of the transition classical → quantum: it is postulated that the evolution of the quantum system is given by a one-parametric group of unitary automorphisms; the infinitesimal generator has necessarily the form $i \times$ (self adjoint operator), and the parallelism with Classical Mechanics forces the group to be one generated by a constant multiple of the quantized Hamilton function (it remains the problem of find that quantized operator, a problem we take for solved). Passing the time evolution of the states to that of operators (Heisenberg representation), the evolution law would be $[\hat{H}, \hat{a}_i] = i\hbar \hat{a}_i / dt$, in analogy with the equation of the evolution for the classical magnitudes: $da_i / dt = \{ H, g \}$ (along each trajectory).

The problem is the non-existence of a function which could be called 'time' in the formalism of the Classical Mechanics (see [7]), although there exist a time of travel along each trajectory of a given mechanical system. To introduce a 'time' function, in general it is needed the addition of a dimension to the given configuration space and then to impose a constraint by a non univocally defined procedure. However, in case of conservative systems, for each lagrangian manifold of a complete integral of the Hamilton–Jacobi there is a 'time' function that parameterizes any particular solution curve within the lagrangian manifold; except for the systems free of forces (geodesic), this time is not proportional to the 'action' function in the lagrangian manifold, so that front waves of the action does not move to a constant temporal rate; the 'time' which measures the movement of the wave fronts is another one: the quotient of action by energy. In the foundational memory of Schrödinger [17] the first part is dedicated to the Hamiltonian analogy between Mechanics and Optics; it seems that Schrödinger is carried
away by the intuition of absolute time and he use the ‘t’ with two different meanings: in the formulae (3), (9), t is the time that parameterizes the trajectories while in formulae (5), (6), t is the quotient action/energy. With this second ‘time’ the wave fronts of the action move at a constant rate.

In a subsequent paper, we will study the nature of ‘time’ in Classical, Undulatory and Quantum Mechanics in conservative systems [8].

7. Final remarks

The method of quantization that we have presented shows up a bridge which links Classical Mechanics with Quantum Mechanics. Our rules of quantization are canonically stated without previous mention to coordinate systems. The examples that we have given in the text and the subsequent comments are illustrations of this general procedure. In addition, they can serve to relate our method with another ones.

The quantization method we have exposed assigns to each ‘classical magnitude’ a a differential operator $\hat{a}$ on the configuration space $M$. Even if the tensor $a$ is real and symmetric, the operator $\hat{a}$ on $L^2(M)$ may be not self-adjoint. If one wishes to establish a Correspondence Principle which assigns to each real classical magnitude a self-adjoint operator, $\hat{a}$ must be replaced by $(\hat{a} + \hat{a}^+) / 2$; when the tensor $a$ is real, the differential operators $\hat{a}$ and $(\hat{a} + \hat{a}^+) / 2$ have the same symbol: they differ by a lower order operator. As an example, when $a$ is a differential 1-form, we get $\hat{a} = -i\hbar \text{ grad } a$, which is self-adjoint if and only if the vector field $u = \text{ grad } a$ is conservative (i.e.: if the flux of $u$ preserves the volume form defined on $M$); the replacement of $\hat{a}$ by $(\hat{a} + \hat{a}^+) / 2$ means modifying $u$ to be $u + \frac{1}{2} \text{ div } u$.

On the other hand, the condition of selfadjointness can be substituted by normality (commutation of an operator with its adjoint) if complex values in the measures are admitted (see for example Penrose [18], p 539).

Although operators in quantum mechanics generally are discontinuous, in the most simple case of complete systems of pairwise commuting continuous operators, the corresponding pure states are points of the spectrum of the algebra generated by that system. The Gelfand–Naimark theorem applies to commutative and stable by invariance Banach algebras whose elements are normal but not necessarily self adjoint (see [19, pp 271–2]).

As an example, let us consider $M = \mathbb{R}^3$ with the Euclidean metric $T_2$. By using spherical coordinates, we have $T_2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2(\theta) d\varphi^2$. The change of coordinates $(r, \theta, \varphi, t, \psi)$ on $T^*\mathbb{R}^3$ to the coordinates $(r, \theta, \varphi, p_r, p_\theta, p_\varphi)$ on $T^*\mathbb{R}^3$ is given by the relations $p_r = r \dot{r}$, $p_\theta = r \dot{\theta}$, $p_\varphi = r^2 \sin^2(\theta) \dot{\varphi}$.

Functions $p_r, p_\theta, p_\varphi$ are the ‘classical magnitudes’ associated with tensors $dr, r^2 d\theta^2$ and $r^2 \sin^2(\theta) d\varphi^2$, respectively. The gradients of these 1-forms with respect to the metric $T_2$ are the vector fields $u_r = \partial / \partial r$, $u_\theta = \partial / \partial \theta$, and $u_\varphi = \partial / \partial \varphi$; after product by $-i\hbar$, they give the momentum operators

$$\hat{p}_r = -i\hbar \frac{\partial}{\partial r}, \quad \hat{p}_\theta = -i\hbar \frac{\partial}{\partial \theta} \quad \text{and} \quad \hat{p}_\varphi = -i\hbar \frac{\partial}{\partial \varphi}.$$  

Of those operators, only the last one is self-adjoint, because $\partial / \partial \varphi$ is conservative, but $\partial / \partial r$ and $\partial / \partial \theta$ are not. The self-adjoint operators associated with the momenta are

$$\frac{1}{2}(\hat{p}_r + \hat{p}_r^+) = -i\hbar \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \quad \text{and} \quad \frac{1}{2}(\hat{p}_\theta + \hat{p}_\theta^+) = -i\hbar \left( \frac{\partial}{\partial \theta} + \frac{1}{2} \cot(\theta) \right).$$

These momentum operators modified to become self-adjoint can be found in the literature (see, for example, [2], p 103). In this case, the commutation rules are still valid because the divergence of $\partial / \partial r$ depends only on $r$ and that of $\partial / \partial \theta$ depends only on $\theta$.

In arbitrary coordinates, the substitution of operators $\hat{p}$’s by its associated self-adjoint can cause the lost of commutativity.

It is a quite important fact of the method of quantization presented in this work that the operator associated with the kinetic energy $T$ is $\hat{T} = -(\hbar^2 / 2) \Delta$ (for completely arbitrary manifolds endowed with a non-singular metric of any signature); $\Delta$ is always self-adjoint, since the formula $\Delta = \text{ div} \cdot \text{ grad}$, valid for functions, is the particularization to 0-forms of the general formula $\Delta = \delta d + d \delta$ on hemisymmetric tensors, where the codifferential $\delta$ is $d^\ast$ (for the scalar product of exterior forms on $M$ associated with the metric and orientation given on $M$).

The formula $\hat{T} = -(\hbar^2 / 2) \Delta$ is commonly used, but not always (see, for example, formula (5.2) in [2]). Anyway we do not know any reference where it is derived from a general quantization method.

For each second order symmetric tensor $a = A_{\alpha \beta} dx^\alpha dx^\beta$, the corresponding classical magnitude is $\hat{a} = A_{\alpha \beta} \hat{x}^\alpha \hat{x}^\beta = A_{\alpha \beta} g^{\alpha \gamma} g^{\beta \delta} \hat{\rho}_\gamma \hat{\rho}_\delta = A_{\alpha \beta} \hat{\rho}_\alpha \hat{\rho}_\beta$, the associated vertical differential operator is

$$A = -\hbar^2 A_{\alpha \beta} \frac{\partial^2}{\partial \hat{x}^\alpha \partial \hat{x}^\beta}.$$
and the differential operator related by quantization is

\[ \hat{a} = - \hbar^2 \mathcal{N} \left( \frac{\partial^2}{\partial x^i \partial x^j} - \Gamma^i_{jk} \frac{\partial}{\partial x^j} \right) \tag{7.1} \]

That formula is valid in general. For instance, as tensor \( a \) can be taken the Ricci tensor, Maxwell stress tensor, etc.

The corresponding self-adjoint operator would be \( \frac{1}{2} (\hat{a} + \hat{a}^\dagger) \). For a real tensor \( a \), the formula for the adjoint of \( \hat{a} \) is

\[ \hat{a}^\dagger = \hat{a} - 2 \hbar \text{ div } a^\dagger - \hbar^2 \text{ div } a \cdot a' \tag{7.2} \]

where \( a' \) is the contravariant expression of the tensor \( a \).

This formula holds for arbitrary metric \( T_2 \) and the corresponding Levi-Civita connection \( \nabla \). The verification of (7.2) is a direct computation which is simplified by choosing the coordinates in such a way that the determinant of the metric matrix is 1 (this is always possible locally).

An interesting consequence is that the necessary and sufficient condition for a second order tensor \( a \) to have a self-adjoint quantization \( \hat{a} \) is that \( \text{div } a' = 0 \). For instance, the Einstein tensor and the Maxwell tensor in the vacuum have self-adjoint quantizations (for the Levi-Civita connection).

As a further example, we will compute quantization of third order polynomials in the momenta. We follow the same steps of section 3, except that now equation (3.1) is replaced by the following one (which displays some additional terms)

\[ x^j = x^j \hat{f} + \hat{x}^j \left( 1 + \frac{1}{2!} \Gamma^j_{rs} (x_0) \hat{x}^s \hat{x}^r \right) - \frac{1}{3!} \left( \Gamma^j_{rs} (x_0) \hat{x}^s \hat{x}^r \hat{x}^v \right) - \frac{1}{4!} \Gamma^j_{rs} (x_0) \hat{x}^s \hat{x}^r \hat{x}^v \hat{x}^w - \ldots, \tag{7.3} \]

where the \( \Gamma^i_{rs} \) are the Christoffel symbols of the connection and we inductively define

\[ \Gamma^j_{rs...yz} := \frac{1}{N} \mathcal{P} \left( \frac{\partial \Gamma^j_{rs...v} \partial}{\partial x^v} - \Gamma^j_{rv...yz} - \Gamma^j_{rv...z} \Gamma^v_{yz} - \cdots - \Gamma^j_{rv...} \Gamma^v_{yz} \right), \tag{7.4} \]

\( N \) being the number of indexes in the list \( \{ rsw \cdots yz \} \) and \( \mathcal{P} \) the sum of all the cyclic permutations of the mentioned indexes. For further details, see [11].

By using (7.3) and (7.4) we get, for instance, the quantization of monomials till third order:

\[ \hat{p}_j = - i \hbar \hat{p}_j - \hbar^2 (\hat{p}_j^2 - \hat{p}_j^2) - \Gamma^j_{jk} \frac{\partial}{\partial x^j} \] (already described in the text) and

\[ \hat{p}_j \hat{p}_k = i \hbar \left( \frac{\partial \hat{p}_j \hat{p}_k}{\partial x^j \partial x^k} \right) : \mathcal{P} \left( \frac{\partial \hat{p}_j \hat{p}_k}{\partial x^j \partial x^k} \right) \] (here, as above, \( \mathcal{P} \) denotes the sum over all the cyclic permutations of \( \{ j, k, \ell \} \)).

In the case of a flat metric and its Levi-Civita connection, we can use cartesian coordinates to get the expression for the adjoint of the quantized third order symmetric covariant tensor \( a \):

\[ \hat{a}^\dagger = \hat{a} - 3 i \hbar \text{ div } a' - 3 \hbar^2 \text{ div } a' + i \hbar^3 \text{ div } a' \] (7.6)

where \( a' \) is the contravariant form of \( a \).

In this way, for order 3, it holds, as in the second order case, that \( \hat{a} \) is self-adjoint if and only if \( \text{div } a' = 0 \).

For arbitrary metric, and the corresponding Levi-Civita connection, the formula (7.6) still holds. The verification is an involved computation. We think that there is an analogous formula in arbitrary order, but we have not yet a general proof.

Our method offers a solution to the old problem of ordering in the operators \( p, q \), in arbitrary coordinates. For a flat metric, the formulas for tensors of arbitrary order analogous to (7.2) and (7.6) can be obtained without difficulty by using cartesian coordinates. Once obtained, these formulas can be used in arbitrary coordinates.

This is a very important characteristic of presenting the method in an intrinsic way from the beginning.

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