Geometric aspects of the quantization of a rigid body

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Published in B. Kruglikov, V. Lychagin, E. Straume:
Differential Equations – Geometry, Symmetries and Integrability,
Proceedings of the 2008 Abel Symposium, Springer, 275-285.

Abstract

In this paper we review our results on the quantization of a rigid body. The fact that the configuration space is not simply connected yields two inequivalent quantizations. One of the quantizations allows us to recover classically double-valued wave functions as single valued sections of a non-trivial complex line bundle. This reopens the problem of a physical interpretation of these wave functions.

1 Introduction

The idea of writing quantum mechanics in a coordinate-free way circulated among physicists and mathematicians as a natural consequence of the general relativity principle. One of the main features of quantum mechanics is that it must contain, according to Dirac's ideas, a correspondence with classical mechanics. Having symplectic mechanics at hand, it was natural to formulate a correspondence principle between classical symplectic mechanics and quantum mechanics that associates a self adjoint operator on a Hilbert space with every quantizable classical observable [13, 21]. This is the heart of what has been called the Geometric Quantization (GQ for short).

The above theory proved to be useful in some physically simple situations, but showed to have a number of drawbacks, discussed in detail in Section 2.

The aim of this paper is to discuss some features of a recent geometric approach to quantum theory, the Covariant Quantum Mechanics (CQM for short). The CQM (introduced by Jadczyk and Modugno [10] and further developed in [1, 11, 12, 15, 16, 17, 19, 23, 25]) has two distinguished features with respect to GQ: on one hand, it is simpler, because it deals only with quantum particles in a given gravitational and electromagnetic field, so loosing the generality of GQ; on the other hand, it is more complete, because it naturally incorporates time in a covariant way.

In Section 3 we describe the main features of CQM. In particular we will see that its greater conceptual simplicity implies weaker existence conditions than those of GQ [25]. Moreover, the algebra of quantizable observables is naturally selected from the geometric structures of the theory itself [10, 15, 19]. Finally, it can be proved [11] that the energy operator is characterized as the unique second order covariant operator on the appropriate space. This implies that all possible non-linear modifications of the Schrödinger equation are not invariant with respect to time-dependent changes of coordinates.

In Section 4 we will focus on the quantum theory of a rigid body in the framework of CQM. We remark that the main application of this theory is quantum mechanics of moleculae [9]. Indeed, moleculae also have vibrational motions, but they hold at a much higher energy than rotational and translational motions, and can be dealt with separately.

We show that there are two possible choices for the quantum structure. For one of them wave functions are sections of a trivial bundle, whereas for the other one they are sections of a non-trivial bundle. Accordingly, there are two energy operators, each of which operates on sections of one of the two bundles. We recall that the spectrum of the energy operator represents the physically allowed values of the corresponding quantum observable (see [4], for example). We computed the spectrum of the energy operator in several situations (zero electromagnetic field (free rigid body), magnetic monopole, constant electric field (Stark effect)), obtaining two families of eigenfunctions and eigenvalues. One of them corresponds to the non-trivial bundle, and is parametrized by half-integers.

The above solutions were discovered in the very beginning of the development of quantum mechanics (see *e.g.* [3]), but were classically discarded due to 'lack of continuity' (see, *e.g.*, [4, 14]). Indeed, using Euler angles as coordinates on the rotational part of the rigid body configuration space, these solutions turn out to be double-valued functions. However this is not fully true, because sections of non-trivial bundles *are* indeed continuous and single-valued.

In a sense, our results show that those sections exist due to a geometric phase effect in quantum mechanics of rigid bodies which is analogous to the Aharonov-Bohm effect. Although experiments seem to show no evidence of these solutions in nature, other reasons than continuity should be found in order to justify the fact that they do not play any role.

2 Geometric Quantization

In this section we will briefly recall the GQ setting.

The classical setting in GQ is based on a symplectic manifold (M, ω) with Hamiltonian H. The manifold M models the classical phase space, and the classical observables are real functions on M.

The quantum setting in GQ is based on a Hilbert space $\mathcal{H}$ of quantum states. The quantization is a linear map

$$\mathcal{Q} \colon \mathcal{O} \subset \mathcal{C}^\infty(M) \to \mathrm{Herm}(\mathcal{H})$$

fulfilling

$$[\mathcal{Q}(f), \mathcal{Q}(g)] = -i\hbar \mathcal{Q}(\{f, g\}), \quad \mathcal{Q}(1) = \mathrm{Id}_{\mathcal{H}}\,.$$

Here, $\mathrm{Herm}(\mathcal{H})$ is the set of Hermitian operators on $\mathcal{H}$. Note that quantization is always defined on a subspace $\mathcal{O} \subset \mathcal{C}^\infty(M)$. This is due to some physical restrictions. For instance, if $M = T^*P$ and P is the configuration space of a particle, then quantizing all of $\mathcal{C}^\infty(T^*P)$ would imply the possibility of localizing any observable around a point with arbitrary precision, which is forbidden by Heisenberg's uncertainty principle. Another problem is the irreducibility of the representation map $\mathcal{Q}$, which is sometimes broken by the full set of observables $\mathcal{C}^\infty(M)$ (Groenewold–Van Hove's no-go theorem, [7]).

The problem of constructing a quantum theory from the classical setting is solved as follows. First of all we require the existence of *pre-quantization structures*, *i.e.*

- a complex Hermitian line bundle $L \to M$, whose sections $\psi \colon M \to L$ are interpreted as wave functions;

- A Hermitian connection ∇ on $L \to M$ such that its curvature $R[\nabla]$ fulfills the equation $R[\nabla] = i\frac{1}{\hbar}\omega \otimes \mathrm{Id}_L$.

The existence of such structures implies that M and ω have to satisfy certain topological conditions (Kostant–Souriau theorem), namely:

$$[\frac{1}{\hbar}\omega] \in i(H^2(M, \mathbb{Z})) \subset H^2(M, \mathbb{R}),$$

where i is the map induced in cohomology by the inclusion $i \colon \mathbb{Z} \hookrightarrow \mathbb{R}$. If the above condition is fulfilled then

- $i^{-1}([\omega]) \subset H^2(M, \mathbb{Z})$ parametrizes line bundles;

- $H^1(E,\mathbb{R})/H^1(E,\mathbb{Z})$ parametrizes connections which satisfy the above condition on the curvature.

Summarizing, by a well–known theorem of algebraic topology, pre-quantization structures are parametrized by $H^1(M,U(1))$.

The Hilbert space of quantum states is then defined as the L^2-completion of the space of compactly supported wave functions. For $f \in \mathcal{O} \subset \mathcal{C}^\infty(M)$ the Hamiltonian vector field $X_f : M \to TM$ is lifted to a ∇-horizontal vector field $\tilde{X}_f : L \to TL$. The pre-quantization maps any observable $f \in \mathcal{C}^\infty(M)$ to the operator $\mathcal{Q}(f)$ defined by

$$\mathcal{Q}(f)(\psi) := i\hbar \tilde{X}_f \cdot \psi.$$

It remains to define the subset $\mathcal{O}$. This is usually accomplished by choosing a polarization in M, *i.e.* a Lagrangian subbundle $P \subset TM$ with further hypotheses (like Frobenius integrability, see [26] for example). Then, the elements of $\mathcal{O}$ are functions which are constant along the leaves of the polarization, and the corresponding Hilbert space is constructed from compactly supported wave functions $\psi : M \to L$ which are covariantly constant along the polarization P:

$$\nabla|_P \psi = 0.$$

The fact that not all symplectic manifolds admit polarizations amounts to imposing stronger topological conditions on M and P. See [20, 26] for more details.

It may happen that $H \notin \mathcal{O}$. In such a case a problem for quantizing the energy arises; this is usually solved by means of the Blattner-Kostant-Sternberg method [20]. This is equivalent to defining a (trivial) bundle of Hilbert spaces $\mathcal{H} \times \mathbb{R} \to \mathbb{R}$ and considering the flow of the Hamiltonian vector field X_H as a time-dependent family of bundle automorphism. The quantization of H is then achieved as the time derivative at $t = 0$ of the above family of operators. It has been recently shown [6] that the flow of X_H can also be interpreted as the parallel transport of a connection on the Hilbert bundle. Hence deriving the flow of X_H produces the covariant derivative associated with the connection.

3 Covariant Quantum Mechanics

In CQM "covariance" is regarded as explicit independence of fundamental laws with respect not only to observers and coordinates but also to units of measurement as well.

The classical framework for one particle of mass $m \neq 0$ and charge q is represented by a fibred manifold $t\colon E \to T$, where T is a one-dimensional affine space modelling time, and E is an $n{+}1$-dimensional manifold modelling spacetime. A motion is a section $s\colon T \to E$. The classical phase space is the first jet space J^1E. An observer is a section $o : E \to J^1E$. We use local coordinates (x^0) on T, (x^0, x^i) on E and the induced coordinates (x^0, x^i, x^i_0) on J^1E.

We postulate the following geometric structures:

- a spacelike Riemannian metric g on E, *i.e.*, a Riemannian metric on the fibres of spacetime;
- a connection Γ on $TE \to E$, representing the gravitational field, which is compatible with the fibring t and the metric g;
- a closed two-form F on E, representing the electromagnetic field.

Thus, Γ is determined by g only partially, due to the degeneracy of the metric along "horizontal" directions.

The above structures can be naturally encoded into a 2-form Ω on J^1E

$$\Omega \equiv \Omega(g, \Gamma, F) = \Omega(g, \Gamma) + \frac{q}{2m} F, \tag{1}$$

where $\Omega(g, \Gamma)$ is induced by g, Γ and the contact structure of J^1E via an algebraic operation. Its coordinate expression is

$$\Omega(g, \Gamma) = g_{ij}(dx^i_0 - (\Gamma^i_{\lambda h} x^h_0 + \Gamma^i_{\lambda 0}) dx^\lambda) \wedge (dx^i_0 - x^i_0 dx^0) \tag{2}$$

(the index λ runs from 0 to n). Conservation laws of classical mechanics require that Ω be closed; indeed, later this property is also a necessary consistency condition for the quantum theory. The closure of Ω turns out to be equivalent to a certain symmetry property of the curvature tensor of Γ. It can be proved that $dt \wedge \Omega \wedge \Omega \wedge \Omega \neq 0$. Thus, (Ω, dt, J^1E) is a *cosymplectic manifold* [1] (see *e.g.* [2] for more details).

Note that the cosymplectic form Ω encodes all dynamical structures. This is an important difference between CQM and GQ. In particular, it can be proved (see, *e.g.*, [19]) that Ω admits "horizontal" potentials Θ, i.e. potentials valued in T^*E . Thus, by choosing an observer o, we can write a potential Θ of Ω as

$$\Theta = -H + P = -\Big(\frac{1}{2} m g_{ij} x^i_0 x^j_0 - A_0\Big) dx^0 + (m g_{ij} x^j_0 + A_i) dx^i, \tag{3}$$

[1]This definition is due to A. Lichnerowicz.

where H is the observed Hamiltonian, P is the observed momentum and $A_0 dx^0 + A_i dx^i$ is the observed potential of both the gravitational and the electromagnetic fields.

In this framework we can develop a Hamiltonian stuff including non standard results. In particular, the phase functions $f : J^1E \to \mathbb{R}$ can be lifted to phase vector fields $X_f : J^1E \to TJ^1E$. Even more, these vector fields X_f are projectable to vector fields of spacetime if and only if the phase functions f are second order polynomials in the velocities whose leading coefficients are proportional to g through a real function f^0 of spacetime, i.e. if and only if their coordinate expression is of the type

$$(4) \qquad f = f^0 g_{ij} x_0^i x_0^j + f^i g_{ij} x_0^j + \breve{f}\,, \qquad \text{with} \qquad f^0, f^i, \breve{f} \colon E \to \mathbb{R}.$$

Indeed, these *"special quadratic phase functions"* constitute a Lie algebra, which is different from the Poisson Lie algebra [12]. This Lie algebra includes energy, momentum and position functions and treats them on the same footing.

Quantum structures are postulated in a way which is partially similar to that of GQ.

The starting assumption of CQM is a *quantum bundle* defined as a complex line bundle $L \to E$. Then, CQM postulates a Hermitian connection ∇ on the pullback L^1 of the quantum bundle over the phase space J^1E, with fulfills two conditions:

- the curvature of ∇ is proportional to Ω according to the equality

$$R[\nabla] = i\frac{m}{\hbar}\Omega \otimes \mathrm{Id}_{L^1},$$

- the covariant differential of a quantum section ψ is "horizontal", i.e. valued in T^*E. This property of ∇ is allowed by the property of Ω to admit horizontal potentials. Indeed, the quantum connection C can be regarded as a *distinguished* family of Hermitian connections of the quantum bundle parametrized by the observers $o : E \to J^1E$.

Thus, there are two main differences of the postulates of CQM with respect to GQ. In CQM the line bundle is assumed to be based on spacetime E and not on the phase space J^1E. On the other hand, CQM needs to assume the quantum connection ∇ on the bundle L^1 in order to link ∇ with Ω, which lives on the phase space J_1E. Clearly, in CQM the topological conditions of Konstant-Souriau's theorem have to be fulfilled on E.

In CQM all further geometric quantum structures and the quantum dynamics are derived from the quantum connection by means of a covariant procedure. The requirement of covariance leads us to a method of projectability in order to get rid of observers (which are encoded in the quantum connection); in a sense, this method replaces successfully the search for polarizations of GQ.

The Schrödinger operator S can be derived from the quantum connection ∇ by several geometric methods implementing the criterion of projectability and even more it is uniquely determined by the requirement of covariance [11]. In coordinates we obtain

$$\begin{aligned} (5) \quad S(\psi) = \Big(& \frac{\partial}{\partial x^0} - iA_0 + \frac{1}{2\sqrt{|g|}}\frac{\partial\sqrt{|g|}}{\partial x^0} - i\frac{k}{2}r \\ & - i\frac{\hbar}{2m} g^{hk}\big((\frac{\partial}{\partial x^h} - iA_h)(\frac{\partial}{\partial x^k} - iA_k) + \Gamma_{hk}^{l}(\frac{\partial}{\partial x^l} - iA_l)\big)\Big)\psi, \end{aligned}$$

where r is the scalar curvature of Γ and k is a constant. We stress that if we release the hypothesis of invariance with respect to units of measurement (for instance, by assuming a distinguished length), then further terms are allowed in the expression of the Schrödinger operator; for instance terms proportional to $|\psi|^2$ may appear, so yielding well known non-linear generalizations of the Schrödinger operator.

Also the quantizable observables and the corresponding quantum operators can be achieved by means of the projectability criterion. One starts by classifying the projectable Hermitian vector fields of the quantum bundle. It can be proved that these vector fields constitute a Lie algebra which is naturally isomorphic to the Lie algebra of special quadratic phase functions, according to the formula [12]

$$f \mapsto \tilde{X}_f = f^0\,\partial_0 - f^i\,\partial_i + i(f^0\,A_0 - f^i\,A_i + \breve{f}) \otimes \mathrm{Id}_L$$

Then, we obtain an injective Lie algebra morphism between the Lie algebra of special quadratic phase functions and the Lie algebra of operators acting on the quantum sections, according to the equality

$$\mathcal{Q}(f)(\psi) := i\hbar\tilde{X}_f \cdot \psi.$$

Indeed, the above results can be applied to energy, momentum and position functions on the same footing. We stress that they are obtained with no further topological conditions on E and that they naturally include the so-called metaplectic correction [20, 26].

Next, the Hilbert bundle $\mathcal{H} \to T$ over time is defined as the L^2-completion of the space of quantum sections $\psi \colon E \to L$ with spacelike compact support. Each section $\hat{\psi} : T \to \mathcal{H}$ can be regarded as a section $\psi : E \to L$ of the quantum bundle. The quantum states are described by the sections $\hat{\psi}$ of the

Hilbert bundle. Moreover, the Schrödinger operator can be regarded as a connection of this infinite dimensional bundle.

Eventually, we can associate a symmetric operator $\hat{f}$ acting on the sections $\hat{\psi}$ of the Hilbert bundle with each special quadratic phase function f by means of the equality

$$\hat{f}(\psi) = (\mathcal{Q}(f) - i f^0 S)(\psi)\,.$$

This is the quantization procedure of CQM, which deals with all quantizable functions (including energy) on the same footing.

4 Rigid body

Following [5, 17, 18], we treat the classical mechanics of a system of n particles by representing this system as a single particle moving in a higher dimensional spacetime which fulfill the same properties postulated for the standard spacetime. Then we define the rigidity constraint and study its main properties. For this purpose we postulate a flat spacetime.

More precisely, we require E to be an affine 4-dimensional space, $t\colon E \to T$ to be an affine surjective map and g to be a Euclidean metric on $S = \operatorname{Ker} Dt$. Note that VE is naturally isomorphic to $E \times S$. We choose Γ to be the natural flat connection on E, and we can consider different examples of electromagnetic field F on E.

The configuration space for a system of n particles is then

$$E_n = E \underset{T}{\times} \cdots \underset{T}{\times} E \to T.$$

This is endowed with the natural flat connection Γ_n induced by Γ and by the product electromagnetic field $F \times \cdots \times F$ (n times). Analogously, we introduce the vector space $S_n = S \times \cdots \times S$. If the n particles have masses $m_1,\ldots,m_n$, then we define the metric on S_n, or inertia tensor, as

$$I = \mu_1 g + \cdots + \mu_n g,$$

where $\mu_i = m_i/m$ and $m = \Sigma_i m_i$. The above data fulfill the classical axioms of CQM, hence produce a cosymplectic form Ω_n which turns out to be exact, due to the topological triviality of E.

The constraint of rigidity is then defined by

$$R = \{(e_1, \ldots, e_n) \in E_n;\ \|e_i - e_j\| = l_{ij}, i \neq j\},$$

where l_{ij} are positive numbers fulfilling $l_{ij} = l_{ji}$ and $l_{ij} \leq l_{ik} + l_{kj}$.

It can be proved [5, 17, 18] that R is diffeomorphic either to $E \times O(3)$, $E \times SO(3)$ or $E \times S^2$. In all three cases E is the space of center of mass configurations, and the second factor is the space of relative configurations. Intuitively, relative configurations can be thought of as if particles either 'fill' the space, lie in a plane, or are aligned. From now on we only consider the case where R is diffeomorphic either to $E \times O(3)$ or to $E \times SO(3)$. Moreover, the former case can be reduced to the latter because any of the two connected components of $E \times O(3)$ is diffeomorphic to $E \times SO(3)$, and motions starting in one of the two connected components remain there forever.

The natural inclusion $R \hookrightarrow E_n$ allows us to define, by pullback, a connection Γ_r and an "electromagnetic field" F_r on R. It can be proved that these constrained data fulfill the classical axioms of CQM. Moreover, the induced form Ω_r turns out to be exact, hence the quantum structure postulated by CQM exists.

Both the configuration space E_n and the rigidity constraint fulfill the same axioms as the classical one-particle theory. For this reason the CQM machinery can be applied, and a quantum theory for the rigid body can be formulated.

Let us compute all possible inequivalent quantum structures on R. Observe that $H^1(SO(3), U(1)) = \mathbb{Z}_2$. Then we have the following theorem [24]; see also [22, 17].

1 Theorem. *There are two inequivalent quantum structures:*

$$L^+ = R \times \mathbb{C} \to R, \qquad L^- \not\simeq R \times \mathbb{C} \to R$$

Both L^+ and L^- admit a unique flat Hermitian connection, that can be naturally deformed with dynamical terms in order to obtain the quantum connections ∇^+ and ∇^-:

It is interesting to observe that the above line bundles (as well as their flat connections) are obtained as vector bundles which are associated with the $\mathbb{Z}_2$-principal bundle $SU(2) \to SO(3)$ by means of the two representations of $\mathbb{Z}_2$ into $\mathbb{C}$.

We stress that the above two quantum structures give rise to two different energy operators with two different spectra. We computed spectra in several examples in [17, 22]; here we will only sketch some results in simple cases.

It is worth to remark that we only compute *rotational* spectra. This means that we only consider rotations of a rigid body around its center of mass, dropping the center-of-mass component of the energy operator. This idea is physically justified by remembering that the most important application of our model is to the study of quantum dynamics of moleculae. In that case rotational and translational phenomena are located on very different energy sectors, and the translational spectrum of moleculae yields a neglectible continuum infrared component [9]. In mathematical terms, we will only compute spectra on the subspace of sections of L^+, L^- which are constant on the center of mass space.

Moreover, we distinguish between three types of rigid body. In fact $SO(3)$ is a Lie group endowed with the left-invariant metric I and the standard bi-invariant Killing metric k. Hence, I can be diagonalized with respect to k. The rigid body is said to be *spherical* if all the three eigenvalues are equal, *symmetric*, or a *top*, if two eigenvalues are equal, *asymmetric* if all the eigenvalues are different. All cases exist in molecular dynamics, *e.g.* CH_4 is a spherical molecula, NH_3 is a symmetric molecula, ...

We have the energy operators $\hat{H}^+$, $\hat{H}^-$ acting respectively on sections of $L^+ \to R$ and $L^- \to R$:

$$(6)\quad \hat{H}^+(\psi^+) = \frac{1}{2}(\Delta^+ + A_0 + kr)(\psi^+), \quad \hat{H}^-(\psi^-) = \frac{1}{2}(\Delta^- + A_0 + kr)(\psi^-),$$

where $\Delta^\pm$ is Bochner Laplacian of $\nabla^\pm$.

2 Theorem ([22]; see also [17]). *In the free (*i.e. $F = 0$*) spherical case the spectrum of $S^\pm$ is the set*

$$E_j^\pm = \frac{\hbar^2}{2I} j(j+1) + k\frac{3\hbar^2}{4I}$$

where

- *E_j^+ is parametrized by $j \in \mathbb{Z}$;*
- *E_j^- is parametrized by $j + 1/2 \in \mathbb{Z}$*

(in other words, j is half integer in the latter case).

Note that $SO(3)$ has constant scalar curvature. This implies that scalar curvature contributes to the spectrum through an overall shift.

Now, choose a splitting $E \simeq T \times P$, where P is a 3-dimensional affine space, and let $o \in P$. A magnetic monopole field is a closed 2-form B on P which is invariant with respect to rotations about o. This means that B is proportional to the volume form on the unit sphere with scaling factor given by the magnetic charge . A magnetic monopole B induces a left-invariant 2-form B on $SO(3)$. Let $q = \sum_i q_i r_i/\|r_i\|$ be the center of charge of the rigid body.

3 Theorem ([22]). *In the spherical case, if $F = B$, then the the spectrum of $S^{\pm}$ is the set*

$$E^{\pm}_{j,l} = \frac{\hbar^2}{2I} j(j+1) - \hbar\nu \frac{\|q\|}{I} l + \nu^2 \frac{\|q\|^2}{2I} + k\frac{3\hbar^2}{4I}$$

where ν is the magnetic charge of the monopole and

- $E^{+}_{j,l}$ *is parametrized by $j, l \in \mathbb{Z}$, $-j \leq l \leq j$;*
- $E^{-}_{j,l}$ *is parametrized by $j + 1/2, l + 1/2 \in \mathbb{Z}$, $-j \leq l \leq j$.*

Note that the existence conditions of quantum structures imply that the magnetic charge ν is quantized.

Other examples of spectral computations have been considered so far.

- Energy spectra for the top and the asymmetric rigid body have been computed in [22] both with $F = 0$ and with a magnetic monopole field. The case of a linear rotor, *i.e.* $R \simeq E \times S^2$, has also been computed (just as an example, CO_2 is a linear molecula).
- We have considered the Stark effect in [17]. Assume a constant (spacelike) electric field $\vec{E}$. The component of F along $SO(3)$ has potential $A_0 = \frac{1}{m}\vec{E} \cdot \mu$, where $\mu = \sum_i q_i r_i$ is the dipole momentum. The spectrum of the energy operator can be computed with the same techniques as in [8], yielding another family of solutions on the non-trivial bundle that are parametrized by half integers.

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