On the geometry of the energy operator in quantum mechanics

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We dedicate this paper to the 70th birthday of Luigi Mangiarotti and Marco Modugno Published in Int. J. of Geom. Meth. Mod. Phys. Vol. 11, No. 07: 1460027

Abstract

We analyze the different ways to define the energy operator in geometric theories of quantum mechanics. In some formulations the operator contains the scalar curvature as a multiplicative term. We show that such term can be canceled or added with an arbitrary constant factor, both in the mainstream Geometric Quantization and in the Covariant Quantum Mechanics, developed by Jadczyk and Modugno with several contributions from many authors.

1 Introduction

One of the problems of quantum mechanical theories is the fact that it is not possible to consistently quantize all physical observables. This fact finds its justification in different ways: the Heisenberg principle forbids the simultaneous localization of position and momenta observables, it is not possible to find an irreducible representation of the space of all polynomials in position and momenta (Groenewold–Van Hove's theorem), etc..

The problem persists in the mathematical models of quantum mechanical theories. Within such models, one of the most developed and successful is Geometric Quantization (GQ for short, see for example [28, 36]). In this theory it is possible to quantize the family of observables which preserve the directions of another distinguished family of observables. The space of such directions is an integrable lagrangian distribution on the phase space, and it is said to be a polarization. For example, in the Schrödinger quantization of particle mechanics it is possible to quantize observables which are linear in the momenta, that is of the form $f^i(x^j)p_i + f_0(x^j)$, since their Hamiltonian vector fields preserve the tangent vectors $\partial/\partial p_i$, which span the so-called vertical polarization. However, the energy is a quadratic function of the momenta and breaks this prescription.

A similar phenomenon occurs in a more recent geometric framework of quantum mechanics that implements the principle of relativity, in the sense of invariance with respect to changes of observer or reference frame. This theory is called Covariant Quantum Mechanics (CQM). It was initiated by Jadczyk and Modugno [6, 7, 8] and later developed by several other authors [2, 11, 12, 22, 23, 24, 25, 26, 27, 31, 34, 35], also with extensions to general relativistic mechanics [14, 15, 17].

In this paper we compare the peculiar ways of quantizing energy in GQ and CQM. In this process we find out interesting geometric features of the covariant energy operator in the two theories. Let us discuss this program more in detail.

In GQ the standard way to quantize the energy in a certain polarization is the socalled Blattner-Kostant-Sternberg method (BKS). This method is applicable to those observables, like the energy, whose Hamiltonian vector fields do not preserve the polarization. One starts with a wave function polarized along the chosen polarization, then both data are dragged by the flow of the energy vector field in order to produce new wave functions polarized along infinitesimally close polarizations. Under suitable conditions the wave functions polarized with respect to the original and the new polarizations are related by the so called BKS-pairing. By means of it one is able to express the change induced by dragging the wave function as a one parameter family of wave functions polarized along the original polarization. The zero time derivative of this family of wave functions gives, by definition, the action of the quantized energy operator on the initial wave function. This yields the method for obtaining a 'correct' quantization of energy in GQ.

In CQM we define two quantum operators connected with energy: 1 - the Lie derivative of wave functions with respect to the Hamiltonian vector field of the energy; 2 a Schrödinger operator obtained from a Lagrangian which is uniquely characterized by covariance requirements. Then, the quantization of energy is the only linear combination of the above operators that does not depend on time derivatives. Section 2 contains a summary of CQM with an emphasis on concepts and formulae which are relevant to the definition of the energy operator.

In GQ the wave functions are defined as *half-forms*, *i.e.* sections of a complex line bundle twisted by the square root of the bundle of volume forms normal to the polarization. This enables one to integrate the natural pairing between any two half-forms. Half-forms were introduced in [1]. Initially, [6, 7, 8] CQM also used half-forms for defining wave functions, then they have been dropped by assuming a Hermitian metric with values in densities [11, 12, 13]. In order to ease the comparison with GQ, here we use CQM as originally formulated with half-forms.

If we wish to compare GQ and CQM we should make further assumptions on GQ's

general setting. In particular, such a comparison makes sense if we consider systems of particles, possibly with holonomic constraints, in the Schrödinger representation. In other words, we consider a Riemannian manifold M and the symplectic manifold T^*M , and quantize with respect to the vertical polarization, which is generated by the vector fields $\partial/\partial p_i$.

The quantization of energy in GQ and CQM leads to energy operators which differ by a term which is a multiplication operator on the wave function by the scalar curvature of the given spacelike metric. Let us discuss this feature more in detail.

The scalar curvature term first made its appearance in the paper [4], in the context of Feynman path integral approach to quantum mechanics. Several authors have tried to determine the factor in front of the scalar curvature term via path integral, but they have found different results, according to different ways of performing the integral. Similar computations within the BKS approach, together with their relation to path integral, are presented in [28, 36] and exhibit a scalar curvature multiplication operator of the form

(1)
$$\Psi \mapsto \frac{1}{6}r\Psi,$$

where r is the scalar curvature of the Riemannian metric of the configuration space. It shall be remarked that not all authors in GQ show this term in their computations.

According with CQM, scalar curvature can be added to the Schrödinger operator through its Lagrangian as a constant multiple of the norm of sections of the quantum bundle. The corresponding Euler–Lagrange expressions contain the term

(2)
$$\Psi \mapsto kr\Psi_{\pm}$$

where $k \in \mathbb{R}$. It was proved by covariance arguments that such a Lagrangian is unique [10] and that the corresponding Schrödinger operator is also unique [12] exactly up to the constant factor k in front of the scalar curvature, that remains undetermined.

The main result of this paper (Section 3) is that the scalar curvature operator in GQ is canceled out when one performs the double covariant derivative in the Bochner Laplacian by keeping into account that there is a natural connection on the square root of the vertical polarization. Indeed, polarized sections are of the form $\Psi: \mathbf{M} \to \mathbf{Q} \otimes \sqrt{\wedge^n T^* \mathbf{M}}$ (with a possible dependence on time), where $\mathbf{Q} \to \mathbf{M}$ is a Hermitian complex line bundle and $n = \dim \mathbf{M}$. Since \mathbf{M} is a Riemannian manifold there is a natural connection on the bundle $\wedge^n T^* \mathbf{M} \to \mathbf{M}$. It is natural to assume that in Bochner's Laplacian $g^{ij} \nabla_i \nabla_j$ covariant derivatives are tensor products of the connection on the square root bundle of densities.

On the other hand, a multiplication operator of the type (2) may always be added to the energy operator without violating covariance. To our knowledge there is no evidence in experiments of the presence of the scalar curvature term in the energy operator. In view of our results and of the previous results about the indeterminacy of the constant k we argue that it might be the case that such a term has simply no physical relevance.

2 Covariant Quantum Mechanics

We start with a summary of the classical and quantum theory developed by Jadczyk, Janyška and Modugno. The interested reader may refer, for instance, to [8, 11, 12, 13] for further details.

In CQM 'covariance' includes also independence from the choice of units of measurements. For this reason, we developed a rigorous treatment of spaces uf units of measurement; roughly speaking they have the same algebraic structure of \mathbb{R}^+ , but no distinguished generator over \mathbb{R}^+ [16]. In this paper, we assume the following "positive 1-dimensional semi-vector spaces" over \mathbb{R}^+ as fundamental unit spaces: the space \mathbb{T} of *time intervals*, the space \mathbb{L} of *lengths*, the space \mathbb{M} of *masses*. Moreover, we assume the *Planck constant* to be an element $\hbar \in \mathbb{T}^* \otimes \mathbb{L}^2 \otimes \mathbb{M}$. We refer to a particle with mass $m \in \mathbb{M}$ and charge $q \in \mathbb{T}^* \otimes \mathbb{L}^{3/2} \otimes \mathbb{M}^{1/2}$.

2.1 Classical theory

The spacetime is an oriented (n + 1)-dimensional manifold \boldsymbol{E} (in the standard case n = 3), the absolute time is an affine space associated with the vector space $\boldsymbol{R} \otimes \mathbb{T}$, the absolute time map is a fibring $t : \boldsymbol{E} \to \boldsymbol{T}$. We denote fibred charts of spacetime by $(x^{\lambda}) \equiv (x^0, x^i)$; the corresponding vector fields and forms are denoted by ∂_0 , ∂_i and d^0 , d^i . The tangent space and the vertical space of \boldsymbol{E} are denoted by $T\boldsymbol{E}$ and $V\boldsymbol{E}$. It is easy to check that \boldsymbol{E} is orientable if and only if it is spacelike-orientable; that means, that $\wedge^4 T^*\boldsymbol{E} \to \boldsymbol{E}$ is a trivial line bundle if and only if $\wedge^3 V^*\boldsymbol{E} \to \boldsymbol{E}$ is a trivial line bundle. As usual, $V\boldsymbol{E} := \ker T\boldsymbol{E}$.

A motion is a section $s: \mathbf{T} \to \mathbf{E}$. The phase space is the first jet space of motions $J_1\mathbf{E}$ (see [18, 21] about jet spaces). We denote fibred charts of phase space by $(x^0, x^i; x_0^i)$. The absolute velocity of a motion s is its first jet prolongation $j_1s: \mathbf{T} \to J_1\mathbf{E}$. An observer is a section $o: \mathbf{E} \to J_1\mathbf{E}$ and the observed velocity of a motion s is the map $\nabla[o]s := j_1s - o \circ s: \mathbf{T} \to \mathbb{T}^* \otimes V\mathbf{E}$.

The spacelike metric is a scaled Riemannian metric of the fibres of spacetime $g : \mathbf{E} \to \mathbb{L}^2 \otimes (V^* \mathbf{E} \underset{\mathbf{E}}{\otimes} V^* \mathbf{E})$. Given a particle of mass m, it is convenient to consider the re-scaled spacelike metric $G := \frac{m}{\hbar}g : \mathbf{E} \to \mathbb{T} \otimes (V^* \mathbf{E} \underset{\mathbf{E}}{\otimes} V^* \mathbf{E})$. The spacelike and spacetime volumes are, respectively, the tensor fields (3)

$$\eta \colon \boldsymbol{E} \to \mathbb{L}^3 \otimes \wedge^3 V^* \boldsymbol{E}, \quad \eta = \sqrt{|g|} \check{d}^1 \wedge \check{d}^2 \wedge \check{d}^3, \quad \bar{\eta} \colon \boldsymbol{E} \to \mathbb{T} \otimes \mathbb{L}^3 \otimes \wedge^4 T^* \boldsymbol{E}, \quad \bar{\eta} = dt \wedge \eta,$$

where $|g| = \det(g_{ij})$ and $\check{}$ denotes vertical restriction.

The gravitational field is a time preserving torsion free linear connection on the tangent bundle of spacetime $K^{\natural}: TE \to T^*E \bigotimes_{TE} TTE$, such that $\nabla[K^{\natural}]g = 0$ and the curvature tensor $R[K^{\natural}]$ fulfills the condition $R^{\natural}_{\lambda}{}^{i}{}_{\mu}{}^{j} = R^{\natural}{}_{\mu}{}^{j}{}_{\lambda}{}^{i}$. The 'metricity' condition on K^{\natural} implies that its vertical restriction coincides with the family of Riemannian connections induced by g on the fibres of $E \to T$. This implies that the Christoffel

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symbols with three spacelike indexes are of the type $\Gamma^i_{jk} = -\frac{1}{2} g^{ih} (\partial_j g_{hk} + \partial_k g_{hj} - \partial_h g_{jk})^1$. The *electromagnetic field* is a scaled 2-form $f: \mathbf{E} \to (\mathbb{L}^{1/2} \otimes \mathbb{M}^{1/2}) \otimes \Lambda^2 T^* \mathbf{E}$, such

The electromagnetic field is a scaled 2-form $f: \mathbf{E} \to (\mathbb{L}^{1/2} \otimes \mathbb{M}^{1/2}) \otimes \Lambda^2 T^* \mathbf{E}$, such that df = 0. Given a particle of charge q, it is convenient to consider the re-scaled electromagnetic field $F := \frac{q}{h}f: \mathbf{E} \to \Lambda^2 T^* \mathbf{E}$.

The electromagnetic field F can be "added", in a covariant way, to the gravitational connection K^{\natural} yielding a *(total) spacetime connection* K, with coordinate expression

$$K_{i\,j}^{\,h} = K^{\natural}{}_{i\,j}^{\,h}, \quad K_{j\,0}^{\,h} = K_{0\,j}^{\,h} = K^{\natural}{}_{0\,j}^{\,h} + \frac{1}{2}F^{\,h}{}_{j}, \quad K_{0\,0}^{\,h} = K^{\natural}{}_{0\,0}^{\,h} + \frac{1}{2}F^{\,h}{}_{0}$$

This turns out to be a time preserving torsion free linear connection on the tangent bundle of spacetime, which still fulfills the properties that we have assumed for K^{\natural} .

The spacetime fibration, the total spacetime connection and the spacelike metric, yield, in a covariant way, a 2-form $\Omega : J_1 \mathbf{E} \to \Lambda^2 T^* J_1 \mathbf{E}$ on the phase space, with coordinate expression

(4)
$$\Omega = G_{ij}^0 \left(d_0^i - (K_\lambda{}^i{}_0 + K_\lambda{}^i{}_h x_0^h) d^\lambda \right) \wedge (d^j - x_0^j d^0).$$

This is a cosymplectic form (see [15] and references therein for a deeper discussion on the geometry of these objects), i.e. it fulfills the following properties: 1) $d\Omega = 0$, 2) $dt \wedge \Omega^n : J_1 \mathbf{E} \to \mathbb{T} \otimes \Lambda^n T^* J_1 \mathbf{E}$ is a scaled volume form on $J_1 \mathbf{E}$. Conversely, the cosymplectic form Ω characterises the spacelike metric and the total spacetime connection. Moreover, the closedness of Ω is equivalent to the conditions that we have assumed on K.

There is a unique second order connection [21] $\gamma : J_1 \mathbf{E} \to \mathbb{T}^* \otimes T J_1 \mathbf{E}$, such that $i_{\gamma}\Omega = 0$. We assume the generalised Newton's equation $\nabla[\gamma]j_1s = 0$ as the equation of motion for classical dynamics. Of course the above equation also admits a Lagrangian and a Hamiltonian formulation [26]. The cosymplectic form Ω admits locally potentials of the type $\Theta : J_1 \mathbf{E} \to T^* \mathbf{E}$. It turns out that these potentials are the Poincaré–Cartan forms of the Lagrangians \mathcal{L} that can be obtained as one of the two summands of the splitting $\Theta = \mathcal{L} + \mathcal{P}$, where $\mathcal{L} : J_1 \mathbf{E} \to T^* \mathbf{T}$ and $\mathcal{P} : J_1 \mathbf{E} \to V^* \mathbf{E}$ is the momentum. These components are observer independent, but depend on the chosen gauge of the starting Poincaré–Cartan form. On the other hand, given an observer o, each Poincaré–Cartan component $-\mathcal{H}[o] : J_1 \mathbf{E} \to T^* \mathbf{T}$, which is called the observed Hamiltonian, and the vertical component $\mathcal{P}[o] : J_1 \mathbf{E} \to V^* \mathbf{E}$, which is the observed momentum. We have the coordinate expressions

(5)
$$\mathcal{L} = \left(\frac{1}{2}G_{ij}^{0}x_{0}^{i}x_{0}^{j} + A_{i}x_{0}^{i} + A_{0}\right)d^{0}, \quad \mathcal{P} = (G_{ij}^{0}x_{0}^{j} + A_{i})(d^{i} - x_{0}^{i}d^{0}),$$

and, in a chart adapted to o,

(6)
$$\mathcal{H}[o] = \mathcal{H}_0 d^0 = \left(\frac{1}{2}G^0_{ij}x^i_0x^j_0 - A_0\right)d^0, \quad \mathcal{P}[o] = \mathcal{P}_j d^j = (G^0_{ij}x^j_0 + A_i)d^i,$$

¹Note the difference in sign with respect to the standard convention.

where $A \equiv o^* \Theta$.

The cosymplectic form Ω yields in a covariant way the Hamiltonian lift of functions $f: J_1 \mathbf{E} \to \mathbb{R}$ to vertical vector fields $H[f]: J_1 \mathbf{E} \to V J_1 \mathbf{E}$; consequently, we obtain the Poisson bracket $\{f, g\}$ between functions of phase space. Given an observer, the law of motion can be expressed, in a non covariant way, in terms of the Poisson bracket and the Hamiltonian.

More generally, chosen a time scale $\tau : J_1 \mathbf{E} \to T\mathbf{T}$, the cosymplectic form Ω yields, in a covariant way, the Hamiltonian lift of functions f of phase space to vector fields $H_{\tau}[f] : J_1 \mathbf{E} \to T J_1 \mathbf{E}$, whose time component is τ . In particular, let us introduce the cosymplectic isomorphism $\Omega^{\flat} : T_{\tau} J_1 \mathbf{E} \to T_{\gamma}^* J_1 \mathbf{E}$ between the subspace of vectors in $T J_1 \mathbf{E}$ that project to τ and the subspace of one-forms in $T^* J_1 \mathbf{E}$ that annihilate γ . Let us denote by Ω^{\sharp}_{τ} the inverse of Ω^{\flat}_{τ} . Then we define $H_{\tau}[f] = \Omega^{\sharp}_{\tau}(df - \gamma.f)$. It can be proved that $H_{\tau}[f]$ is projectable onto a vector field $X[f] : \mathbf{E} \to T\mathbf{E}$ if and only if the following conditions hold: i) the function f is quadratic with respect to the affine fibres of $J_1 \mathbf{E} \to \mathbf{E}$ with second fibre derivative $f'' \otimes G$, where $f'' : \mathbf{E} \to I\!\!R \otimes \mathbb{T}$, ii) $\tau = f''$. A function of this type is called a *special phase function* and has coordinate expression of the type

(7)
$$f = \frac{1}{2} f^0 G^0_{ij} x^i_0 x^j_0 + f^0_i x^i_0 + f_0, \quad \text{with} \quad f^0, f^0_i, f_0 : \mathbf{E} \to \mathbb{R}.$$

Note that $f'' = f^0 u_0$, where $u_0 \in \mathbb{T}$ is a time scale. From now on we will assume that f^0 is a constant, even if this assumption could be dropped [8].

The vector space of special phase functions is not closed under the Poisson bracket, but it turns out to be an $I\!R$ -Lie algebra through the covariant *special bracket*

(8)
$$\llbracket f,g \rrbracket = \{f,g\} + \gamma(f'') \cdot g - \gamma(g'') \cdot f.$$

Moreover, the map $f \mapsto X_f$ turns out to be a morphism of Lie algebras; we have the coordinate expression $X_f = f^0 \partial_0 - f^i \partial_i$, where $f^i = G^{ij} f_j$.

2.2 Quantum theory

Let us consider a complex line bundle over spacetime $\mathbf{Q} \to \mathbf{E}$ equipped with a Hermitian metric $h : \mathbf{Q} \times \mathbf{Q} \to \mathbb{C}$. We shall refer to normalised local bases b of \mathbf{Q} and to the associated complex coordinates z; accordingly, the coordinate expression of a *local section* is of the type $\Psi = \psi b$, with $\psi : \mathbf{E} \to \mathbb{C}$.

We consider also the extended line bundle $\mathbf{Q}^{\uparrow} \to J_1 \mathbf{E}$, $\mathbf{Q}^{\uparrow} \coloneqq \mathbf{Q} \times J_1 \mathbf{E}$. A family (or 'system') of connections of \mathbf{Q} parametrised by observers $o: \mathbf{E} \to J_1 \mathbf{E}$ induces, in a covariant way, a connection of \mathbf{Q}^{\uparrow} , which is called *universal* [21, 11]. A characteristic property of the universal connection is that its contraction with any vertical vector field of the bundle $J_1 \mathbf{E} \to \mathbf{E}$ vanishes; in coordinates, $\mathbf{u}_i^0 = 0$.

It is well known that the Picard group Pic(M) of isomorphism classes of complex line bundles over a differentiable manifold M can be identified with the second integral cohomology group $H^2(M,\mathbb{Z})$ by means of the first Chern class mapping

$$c_1 \colon \operatorname{Pic}(M) \xrightarrow{\sim} H^2(M, \mathbb{Z}),$$

such that given a Line bundle $L \to M$ sends its isomorphism class $[L] \in \operatorname{Pic}(M)$ to the first Chern class $c_1(L) \in H^2(M, \mathbb{Z})$. Since $J_1 \mathbf{E} \to \mathbf{E}$ is an affine bundle, it follows from elementary obstruction theory that the map induced on cohomology by pullback along the map $J_1 \mathbf{E} \to \mathbf{E}$ is an isomorphism $(\cdot)^{\uparrow} \colon H^2(\mathbf{E}, \mathbb{Z}) \xrightarrow{\sim} H^2(J_1 \mathbf{E}, \mathbb{Z})$. Therefore, by pulling back complex line bundles on \mathbf{E} to $J_1 \mathbf{E}$ we also get an isomorphism of Picard groups $(\cdot)^{\uparrow} \colon \operatorname{Pic}(\mathbf{E}) \xrightarrow{\sim} \operatorname{Pic}(J_1 \mathbf{E})$.

We say that $\mathbf{Q} \to \mathbf{E}$ is a quantum bundle if there exists a connection $\mathbf{\Psi}: \mathbf{Q}^{\uparrow} \to T^* J \mathbf{E} \underset{J \mathbf{E}}{\otimes} T \mathbf{Q}^{\uparrow}$ on the extended quantum bundle, called a quantum connection, which is Hermitian, universal and whose curvature is $R[\mathbf{\Psi}] = \mathfrak{i} \Omega \otimes \mathrm{id}_{\mathbf{Q}}$. We stress that $\frac{1}{\hbar}$ has been incorporated in Ω through the re-scaled metric G. In a local base b, a quantum connection $\mathbf{\Psi}$ is of the type

(9)
$$\mathbf{u} = \mathbf{u}^{\parallel} + \mathbf{i}\,\Theta \otimes \mathbf{1},$$

where \mathbf{u}^{\parallel} is the flat connection associated with b and Θ is a potential of Ω , the Poincaré– Cartan form. Given an observer o we can also write $\mathbf{u} = \mathbf{u}^{\parallel} + \mathfrak{i} \left(-\mathcal{H}[o] + \mathcal{P}[o]\right) \otimes \mathbf{1}$. We have the coordinate expression

(10)
$$\begin{aligned} \mathbf{u} &= d^{\lambda} \otimes \partial_{\lambda} + d_{0}^{i} \otimes \partial_{i}^{0} + \mathbf{i} \, \mathbf{u}_{\lambda} d^{\lambda} \otimes (z \partial z) \\ &= d^{\lambda} \otimes \partial_{\lambda} + d_{0}^{i} \otimes \partial_{i}^{0} + \mathbf{i} \left(- \left(\frac{1}{2} \, G_{ij}^{0} \, x_{0}^{i} \, x_{0}^{j} - A_{0} \right) d^{0} + \left(G_{ij}^{0} \, x_{0}^{j} + A_{i} \right) d^{i} \right) \otimes (z \partial z). \end{aligned}$$

Given an observer o we have the observed quantum connection $o^* \mathbf{u} : \mathbf{Q} \to T^* \mathbf{E} \underset{\mathbf{E}}{\otimes} \mathbf{Q}$ with coordinate expression $o^* \mathbf{u} = d^\lambda \otimes \partial_\lambda + \mathfrak{i} A_\lambda z d^\lambda \otimes \partial z$ where $A_\lambda d^\lambda = o^* \Theta$.

A quantum connection exists if and only if the cohomology class of Ω is integral; the equivalence classes of quantum bundles equipped with a quantum connection are classified by the cohomology group $H^1(\boldsymbol{E}, U(1))$ [26, 34].

In what follows we assume a quantum bundle equipped with a quantum connection.

Any other quantum object is obtained, in a covariant way, from this quantum structure. The quantum connection is defined on the extended quantum bundle, while we are looking for further quantum objects living on the original quantum bundle. This goal is successfully achieved by a *method of projectability*: namely, we look for objects of the extended quantum bundle which are projectable to the quantum bundle and then we take their projections. Indeed, our method of projectability turns out to be our way of implementing the covariance of the theory; in fact, it allows us to get rid of the family of all observers, which is encoded in the quantum connection (through $J_1 E$).

The quantum connection allows us to take derivatives of sections $\psi \colon E \to Q$. We have the expression:

(11)
$$\nabla_{\lambda}\psi d^{\lambda} \equiv (\partial_{\lambda}\psi - \mathfrak{i}\,\mathfrak{u}_{\lambda}\psi)d^{\lambda} = (\partial_{0}\psi + \mathfrak{i}\,\mathcal{H}_{0}\psi)d^{0} + (\partial_{j}\psi - \mathfrak{i}\,\mathcal{P}_{j}\psi)d^{j},$$

and its 'observed' counterpart

(12)
$$\overset{o}{\nabla}_{\lambda}\psi \equiv (\partial_{\lambda}\psi - \mathfrak{i}A_{\lambda}\psi),$$

where the superscript o means that the covariant derivative is related to the pull-back connection $o^* \mathbf{y}$. Using the splittings of the previous section we may also define

(13)
$$\bar{\nabla}\Psi = (\partial_0\psi + \dot{x}_0^j\partial_j\psi - \mathfrak{i}\mathcal{L}_0\psi)d^0 \otimes b, \qquad \stackrel{\vee}{\nabla}\Psi = (\partial_j\psi - \mathfrak{i}\mathcal{P}_j\psi)\check{d}^j \otimes b.$$

Furthermore, given an observer o we define the observed quantum Laplacian of $\Psi \in \mathcal{S}(\mathbf{Q})$ to be the section $\overset{o}{\Delta}\Psi = \bar{G}(\check{\nabla}^{o}\check{\nabla}^{o}\Psi)$ with coordinate expression in adapted coordinates

$$\overset{o}{\Delta}\Psi = G^{hk} \big((\partial_h - \mathfrak{i} A_h) (\partial_k - \mathfrak{i} A_k) + K_h^{\ l}{}_k (\partial_l - \mathfrak{i} A_l) \big) \psi u^0 \otimes b.$$

J. Janyška [9] has proved that all covariant quantum Lagrangians of the quantum bundle are proportional to

(14)
$$\mathsf{L}[\Psi] = \frac{1}{2} dt \wedge \left(h(\Psi, i\bar{\nabla}\Psi) + h(i\bar{\nabla}\Psi, \Psi) - (\bar{G} \otimes h)(\overset{\vee}{\nabla}\Psi, \overset{\vee}{\nabla}\Psi) + krh(\Psi, \Psi) \right) \eta,$$

with coordinate expression

$$\begin{split} \mathsf{L}[\Psi] &= \frac{1}{2} \big(\mathfrak{i} \left(\bar{\psi} \partial_0 \psi - \psi \partial_0 \bar{\psi} \right) - G_0^{hk} \partial_h \bar{\psi} \partial_k \psi \\ &+ \mathfrak{i} G_0^{hk} A_h (\psi \partial_k \bar{\psi} - \bar{\psi} \partial_k \psi) + \bar{\psi} \psi (2A_0 - G_0^{rs} A_r A_s + kr_0) \big) \sqrt{|g|} d^0 \wedge d^1 \wedge d^2 \wedge d^3 \end{split}$$

where k is an arbitrary real factor and $r = r_0 u^0 : \mathbf{E} \to \mathbb{R} \otimes \mathbb{T}^*$ is the scalar curvature of the spacelike metric G. The corresponding Euler–Lagrange expression is $h^{\sharp}(\mathsf{E}[\Psi]) : \mathbf{E} \to \mathbb{L}^3 \otimes (\mathbf{Q} \bigotimes_{\mathbf{E}} \Lambda^4 T^* \mathbf{E})$, with coordinate expression

(15)
$$h^{\sharp}(\mathsf{E}[\Psi]) = 2\big(\mathfrak{i}\,(\partial_0 - \mathfrak{i}\,A_0 + \frac{1}{2}\,\frac{\partial_0\sqrt{|g|}}{\sqrt{|g|}})\psi + \frac{1}{2}\,G_0^{hk}(\partial_h - \mathfrak{i}\,A_h)(\partial_k - \mathfrak{i}\,A_k)\psi \\ + \frac{1}{2}\,\frac{\partial_h(G_0^{hk}\sqrt{|g|})}{\sqrt{|g|}}(\partial_k - \mathfrak{i}\,A_k)\psi + \frac{1}{2}\,kr_0\psi\big)b\otimes\sqrt{|g|}d^0\wedge d^1\wedge d^2\wedge d^3.\,\Box$$

J. Janyška and M. Modugno have proved a uniqueness-by-covariance result for E [12]. Thus, k remains undetermined in our scheme in contrast with other authors. See Section 3 for a more detailed discussion.

Next, we introduce a way to associate to each quantizable function f a vector field on the quantum bundle Q. More precisely, it is proved [8, 11] that there is a natural Lie algebra isomorphism between quantizable functions and a space of vector fields on Q obtained as follows. Given f there is a unique Hermitian vector field Y^{\uparrow}_{f} on the extended quantum bundle Q^{\uparrow} such that it is projectable to $J_{1}E$, it is Ψ -horizontal and its covariant differential $\nabla[\mathbf{u}]Y^{\uparrow}_{f}$ takes its values in the subbundle $\mathbb{T}^{*} \otimes \mathbf{Q}$, in particular $Y^{\uparrow} = \mathbf{u}(H[f]) + \mathbf{i} f$. The vector field Y^{\uparrow}_{f} turns out to be projectable onto a vector field Y_{f} on the quantum bundle \mathbf{Q} , which is said to be a *quantum vector field*. We have the coordinate expression

(16)
$$Y_f = f^0 \partial_0 - f^j \partial_j + \mathfrak{i} (f^0 A_0 - f^h A_h + f_0) z \partial z,$$

The space of quantum vector fields constitute a Lie algebra; it can be proved that it is naturally isomorphic to the Lie algebra of quantisable functions.

The quantum vector field Y_f acts on the sections Ψ of the quantum bundle via the associated Lie derivative $Z_f := i L_{Y_f}$. This is possible since Y_f is projectable. Note that the Lie derivative of Ψ with respect to $Y = Y^{\lambda}\partial_{\lambda} + Yz\partial z$ is $L_Y\Psi = Y^{\lambda}\partial_{\lambda}\psi - Y\psi$. However, it is not enough to have operators on sections of the quantum bundle, since in view of the probabilistic interpretation of wave functions in quantum mechanics we should be able to compute spacelike integrals of quantum sections. With this aim in mind we are naturally led to the introduction of half-forms. These are geometric objects that can be paired each other in order to yield densities. Such densities can be integrated in order to define a Hilbert space norm on the space of quantum states. Namely, we introduce the bundles over E

(17)
$$\boldsymbol{Q}^{\eta} := \boldsymbol{Q} \otimes \mathbb{L}^{3/2} \otimes \sqrt{\wedge^{3} V^{*} \boldsymbol{E}}, \quad \boldsymbol{Q}^{\bar{\eta}} := \boldsymbol{Q} \otimes \mathbb{T}^{1/2} \otimes \mathbb{L}^{3/2} \otimes \sqrt{\wedge^{4} T^{*} \boldsymbol{E}}$$

whose sections are said to be *half-forms*. Here the square root of an oriented vector space is the vector space whose tensor square is the initial vector space, and the bases of the above square roots are the square roots of the bases of the corresponding spaces, *i.e.* the square roots of the volumes. Note that the square root of the volume element is parallel with respect to the spacetime connection K^{\natural} . We will use the notation $\Psi^{\eta} = \Psi \otimes \sqrt{\eta} = \psi \sqrt[4]{|g|} b \otimes \sqrt{\check{d}^1 \wedge \check{d}^2 \wedge \check{d}^3}$, and analogously for $\Psi^{\bar{\eta}}$. We will also make use of the symbols $\psi^{\eta} = \psi \sqrt[4]{|g|}$ and $v = \check{d}^1 \wedge \check{d}^2 \wedge \check{d}^3$, so that $\Psi^{\eta} = \psi \sqrt[4]{|g|} b \otimes \sqrt{v}$. Note that the vertical Riemannian connection induced by the metric g yields a connection on the bundle $\sqrt{\wedge^3 V^* E} \to E$: indeed, if $f \sqrt{\eta}$ is a section of this bundle, then

(18)
$$\check{\nabla}(f\sqrt{\eta}) = (\partial_i f + \frac{1}{2}\Gamma^j_{ij})\check{d}^i \otimes \sqrt{\eta}.$$

The observed Laplacian can be defined on half-forms using the tensor product of the connection $o^* \mathbf{q}$ with the above Riemannian connection on $\sqrt{\wedge^3 V^* \mathbf{E}}$.

Now, let us define the operator

(19)
$$Z_f(\Psi^{\eta}) := \mathfrak{i} L_{Y_f}(\Psi^{\bar{\eta}}) \otimes \frac{1}{\sqrt{\bar{\eta}}} \otimes \sqrt{\eta}.$$

Note that we cannot compute directly the Lie derivative of $\sqrt{\eta}$ with respect to a non-vertical vector field; so, we are forced to use $\sqrt{\overline{\eta}}$ in an obvious way. Note that we have

(20)
$$L_{Y_f}\sqrt{\overline{\eta}} = \frac{1}{2} \frac{\partial_\lambda(Y_f^\lambda \sqrt{|g|})}{\sqrt{|g|}} \sqrt[4]{|g|} \sqrt{u_0 \otimes d^0 \wedge d^1 \wedge d^2 \wedge d^3}$$

We have the expression

(21)
$$Z_f(\Psi^{\eta}) = i \left(f^0 \overset{o}{\nabla}_0 - f^i \overset{o}{\nabla}_i - i f_0 + \frac{1}{2} \left(\frac{\partial_0 (f^0 \sqrt{|g|})}{\sqrt{|g|}} - \frac{\partial_i (f^i \sqrt{|g|})}{\sqrt{|g|}} \right) \right) (\psi)$$
$$\overset{4}{\sqrt{|g|}} b \otimes \sqrt{v}.$$

In particular, we obtain

(22)
$$Z_{x^{\alpha}}(\Psi^{\eta}) = x^{\alpha}\Psi^{\eta}, \quad Z[\mathcal{P}_j](\Psi) = -i\partial_j(\psi^{\eta})b \otimes \sqrt{v}, \quad Z[\mathcal{H}_0](\Psi) = i\partial_0(\psi^{\eta})b \otimes \sqrt{v}$$

As far as the Euler–Lagrange expression (15) is concerned, we can rewrite it using an observer o. Namely, we have the vector field $X^o = o \lrcorner o^* \lor$ and the equality

(23)
$$h^{\sharp}(\mathsf{E}[\Psi]) = 2\left(i\frac{L_{X^{o}}\Psi^{\bar{\eta}}}{\sqrt{\bar{\eta}}} + \frac{1}{2}\overset{o}{\Delta}\Psi + \frac{1}{2}kr\Psi\right) \otimes \bar{\eta}.$$

The above expression yields an operator on half-forms in a natural way. Indeed the first summand is just the Lie derivative of a half-form and we have the equality

(24)
$$(\stackrel{o}{\Delta}\Psi) \otimes \sqrt{\eta} = \stackrel{o}{\Delta}(\Psi^{\eta})$$

since $\sqrt{\eta}$ is parallel with respect to the connection induced on the half-forms bundle. For this reason we define the *Schrödinger operator* to be the operator **S**

(25)
$$\mathsf{S}(\Psi^{\eta}) = -\frac{i}{2}h^{\sharp}(\mathsf{E}[\Psi]) \otimes \frac{1}{\bar{\eta}} \otimes \sqrt{\eta} = L_{X^o}\Psi^{\eta} - \frac{i}{2}\overset{o}{\Delta}(\Psi^{\eta}) - \frac{1}{2}kr\Psi^{\eta}.$$

Next, we consider the pre-Hilbert functional quantum bundle $H \to T$ over time. This is defined as follows: for each $\tau \in T$ let (26)

 $H_{\tau} := \{ \Psi_{\tau}^{\eta} \colon \boldsymbol{E}_{\tau} \to \boldsymbol{Q}_{\tau}^{\eta} \mid \Psi_{\tau}^{\eta} = \Psi^{\eta}|_{E_{\tau}}, \ \Psi^{\eta} \text{ quantum section with compact support} \}$

where $E_{\tau} = t^{-1}(\tau)$. In other words, the infinite dimensional fibres are constituted by the sections of the quantum bundle at a given time and with compact support. The space H can be given the structure of an F-smooth manifold, in the sense of [5]. The functional quantum bundle also inherits the Hermitian structure:

(27)
$$\hat{h}: \boldsymbol{H} \underset{\boldsymbol{T}}{\times} \boldsymbol{H} \to \mathbb{C}: (\Psi^{\eta}_{\tau}, \Psi^{\eta\prime}_{\tau}) \mapsto \int_{\boldsymbol{E}_{\tau}} h(\Psi^{\eta}_{\tau}, \Psi^{\eta\prime}_{\tau}),$$

which makes it a pre-Hilbert bundle.

The tangent space is defined to be the set $TH := \bigcup_{\Psi_{\tau}^{\eta} \in H} T_{\Psi_{\tau}^{\eta}} H$ where

(28)
$$T_{\Psi_{\tau}}\boldsymbol{H} = \{\zeta_{(\tau,u)} \colon T_{(\tau,u)}\boldsymbol{E} \to T_{(\tau,u)}\boldsymbol{Q} \mid T\zeta_{(\tau,u),e} = V_{e}\Psi_{\tau}^{\eta}\}.$$

In other words, the coordinate expression of $\zeta_{(\tau,u)}$ is $\zeta_{(\tau,u)} = \zeta + \partial_i \psi \dot{x}^i$, where ζ is a complex-valued function on \boldsymbol{E} . Let us recall that any section $\Psi^{\eta} \colon \boldsymbol{E} \to \boldsymbol{Q}$ (which is defined on a tube-like open subset) yields the *F*-smooth section

(29)
$$\hat{\Psi}^{\eta} \colon \boldsymbol{T} \to \boldsymbol{H}, \quad \hat{\Psi}^{\eta}(\tau)(e_{\tau}) = \Psi^{\eta}(e_{\tau});$$

conversely, every F-smooth section of $H \to T$ yields a section Ψ^{η} as above, establishing a bijective correspondence.

A connection on the space \boldsymbol{H} can be introduced as a section $\chi \colon \boldsymbol{H} \times T\boldsymbol{T} \to T\boldsymbol{H}$ which is linear over \boldsymbol{H} and projects onto $\mathrm{id}_{T\boldsymbol{T}}$. A connection χ acts on sections as $\chi(\hat{\Psi}^{\eta}) = \chi \circ \hat{\Psi}^{\eta}$, with coordinate expression $\chi(\hat{\Psi}^{\eta}) = \chi_0(\psi^{\eta})u^0 + \partial_i\psi^{\eta}\dot{x}^i$. The covariant differential of sections is defined by

(30)
$$\nabla[\chi]\hat{\Psi}^{\eta} = T\hat{\Psi}^{\eta} - \chi(\hat{\Psi}^{\eta})$$

with coordinate expression $\nabla[\chi]\hat{\Psi}^{\eta} = \partial_0\psi^{\eta} - \chi_0(\psi^{\eta})u^0$.

It is now obvious that the Schrödinger operator **S** is the covariant differential $\nabla[\chi]$ of a connection χ on the functional quantum bundle; hence, the quantum Lagrangian yields a lift of the quantum connection Ψ of the extended quantum bundle to a connection χ of the functional quantum bundle. The coordinate expression of χ is

(31)
$$\chi_0(\Psi^\eta) = \left(\mathfrak{i} A_0 + \frac{i}{2} \overset{o}{\Delta}_0 + \frac{1}{2} k r_0\right) \Psi^\eta.$$

Let us consider a quantisable function f. The operator Z_f can be defined on sections of the functional quantum bundle in an obvious way. Then

(32)
$$\hat{f} = Z_f - i f^0 \,\lrcorner\, \nabla[\chi]$$

is the unique combination of Z_f and $\nabla[\chi]$ which yields an operator acting on the fibres of the functional quantum bundle. We have the following coordinate expression

(33)
$$\hat{f}(\Psi^{\eta}) = \left(-\frac{1}{2}f^{0}\overset{o}{\Delta}_{0} - \mathfrak{i}f^{j}\overset{o}{\nabla}_{j} + f_{0} - \frac{1}{2}kf^{0}r_{0} - \mathfrak{i}\frac{1}{2}\frac{\partial_{j}(f^{j}\sqrt{|g|})}{\sqrt{|g|}}\right)\Psi^{\eta}.$$

The map $f \mapsto \hat{f}$ is injective. Moreover, \hat{f} is Hermitian. We assume \hat{f} to be the Hermitian quantum operator associated with the quantisable function f. This is our correspondence principle.

2.1 Example. Let us consider an observer o and a time scale u_0 and let us refer to a chart adapted to the observer and to the time scale. Then, the quantum operators associated with the quantisable functions $x^{\alpha}, x_0^i, \mathcal{P}_i, \mathcal{H}_0$ are given, for each $\Psi \in \mathcal{S}(Q)$, by

(34)
$$\widehat{x^{\alpha}}(\Psi^{\eta}) = x^{\alpha}\Psi^{\eta}, \qquad \widehat{\mathcal{P}_{j}}(\Psi^{\eta}) = -i\partial_{j}(\psi^{\eta})b \otimes \sqrt{v},$$

(35)
$$\widehat{\mathcal{H}}_{0}(\Psi^{\eta}) = \left(-\frac{1}{2}G^{hk}\left((\partial_{h} - \mathfrak{i}A_{h})(\partial_{k} - \mathfrak{i}A_{k}) + K_{h}^{l}{}_{k}(\partial_{l} - \mathfrak{i}A_{l})\right)(\psi)$$

$$-A_0\psi - \frac{1}{2}kr_0\psi \bigg) \sqrt[4]{|g|}b \otimes \sqrt{v}. \square$$

The commutator of Hermitian fibred operators on the functional quantum bundle yields a Lie algebra structure. However from the formula

(36)
$$[\hat{f}, \hat{g}] = \widehat{\llbracket f, g \rrbracket} + \left[(g'' \otimes L_{Y_f} - f'' \otimes L_{Y_g}), \mathsf{S} \right].$$

we obtain that the correspondence principle fails to be a Lie algebra morphism exactly on quantisable functions with nontrivial quadratic term.

2.2 Remark. The Feynmann path integral formulation of Quantum Mechanics can be naturally expressed in our formalism; in particular, the Feynmann amplitudes arise naturally via parallel transport with respect to the quantum connection [8]. So the Feynmann path integral can be regarded as a further way to lift the quantum connection Ψ to a functional quantum connection.

2.3 Remark. In the particular case when spacetime is flat, our quantum dynamical equations turns out to be the standard Schrödinger equation and our quantum operators associated with spacetime coordinates, momenta and energy coincide with the standard operators. Therefore, all usual examples of standard Quantum Mechanics are automatically recovered in our covariant scheme.

2.4 Remark. The above procedure can be easily extended to classical and quantum multi-body systems (*e.g.*, the rigid body, see [24, 25]), to particles with spin (Pauli equation [3]), and to a more limited extent to the Einstein relativistic mechanics [14].

3 Energy operator from CQM to GQ

In this section we now restrict ourselves to the case when $\mathbf{E} = \mathbf{T} \times \mathbf{M}$, where \mathbf{M} is an orientable Riemannian manifold. Here, in principle, the theory allows a time-dependent metric, but we will not consider this general situation. Note that $J_1(\mathbf{T} \times \mathbf{M}) = \mathbf{T} \times T\mathbf{M}$. Our task is to assume the same structures of the GQ theory in the case of a particle (or a 'generalized' particle in the case in which dim $\mathbf{M} \neq 3$) and compare the energy operator from CQM with the one obtained in GQ. We will refer to [28] for a detailed derivation of the energy operator in this situation (see p. 120, Section 7.2, or p. 180, Section 10.1 for the case with a nonzero electromagnetic field).

We require the gravitational field to be purely space-like, *i.e.* $K^{\natural_0 h}{}_j = K^{\natural_j h}{}_0 = 0$, $K^{\natural_0 h}{}_0 = 0$; this request is intrinsic in view of the splitting $\boldsymbol{E} = \boldsymbol{T} \times \boldsymbol{M}$ of spacetime. We assume F = 0, even if we could at least consider a nonzero magnetic field in principle.

Then, there is a natural symplectic structure on TM which is the pull-back of the canonical structure on T^*M under the metric isomorphism g^{\flat} . The form Ω reduces to the above symplectic form, and the second-order connection γ is the usual geodesic spray $\gamma: TM \to T^2M$. The classical theory can be completely developed from the previous assumptions.

Since we are in a time independent situation, the CQM theory can be developed by assuming a quantum bundle $Q \to T \times M$ which is the pull-back of a Hermitian complex line bundle $\bar{Q} \to M$. In fact, it can be proved that all quantum bundles are of this form. In the same way, if we consider the line bundle $\bar{Q}^{\uparrow} = \tau_M^* \bar{Q} \to TM$, where $\tau_{\boldsymbol{M}} \colon T\boldsymbol{M} \to \boldsymbol{M}$ denotes the tangent bundle projection, then the extended quantum bundle $\boldsymbol{Q}^{\uparrow} \to \boldsymbol{T} \times T\boldsymbol{M}$ is obtained by pulling back $\bar{\boldsymbol{Q}}^{\uparrow} \to T\boldsymbol{M}$ to $\boldsymbol{T} \times T\boldsymbol{M}$. Moreover, any quantum connection $\boldsymbol{\Psi}$ on $\boldsymbol{Q}^{\uparrow} \to \boldsymbol{T} \times T\boldsymbol{M}$ that fulfills the curvature identity $R[\boldsymbol{\Psi}] = \mathfrak{i} \Omega \otimes \mathrm{id}_{\boldsymbol{Q}}$ is obtained in a two step process. In the first one we consider the connection $\bar{\boldsymbol{\Psi}}^{\uparrow}$ on $\bar{\boldsymbol{Q}}^{\uparrow} \to T\boldsymbol{M}$ obtained by pulling back a Hermitian connection $\bar{\boldsymbol{\Psi}}$ on $\bar{\boldsymbol{Q}} \to \boldsymbol{M}$ and adding to it a suitable constant multiple of the 1-form $(g^{\flat})^*\theta$, where θ is the Liouville form on $T^*\boldsymbol{M}$, see [19] for the precise details. In the second step, we pull back $\bar{\boldsymbol{\Psi}}$ to $\boldsymbol{Q}^{\uparrow} \to T \times T\boldsymbol{M}$ in order to get the connection $\boldsymbol{\Psi}$. It is clear that $\bar{\boldsymbol{Q}}^{\uparrow} \to T\boldsymbol{M}$ and $\bar{\boldsymbol{\Psi}}^{\uparrow}$ define a quantum structure in the sense of the standard GQ.

The polarization P that we choose is the vertical one, *i.e.* $P = VTM = \ker \tau_{TM} \subset TTM$ which is locally spanned by the vector fields $\partial/\partial \ddot{x}^i$. We have the canonical isomorphism $VTM \simeq TM \times TM = \tau_M^*TM$. We stress that half-forms in CQM and half-forms in GQ in the above setting are the same (up to dependency on time, which in GQ is not explicit). Indeed, the determinant bundle of the polarization P is by definition $K_P = \det(P^\circ)$, where $P^0 \subset T^*TM$ is the subbundle that anihilates $P \subset TTM$. One has the following exact sequence

$$0 \rightarrow \mathbf{P} \rightarrow TT\mathbf{M} \rightarrow \tau_{\mathbf{M}}^*T\mathbf{M} \rightarrow 0,$$

and taking duals we get the exact sequence

$$0 \to \tau_{\boldsymbol{M}}^* T^* \boldsymbol{M} \to T^* T \boldsymbol{M} \to \boldsymbol{P}^* \to 0.$$

This shows that $\boldsymbol{P}^\circ = \tau_{\boldsymbol{M}}^* T^* \boldsymbol{M}$ and therefore

$$K_{\boldsymbol{P}} = \det(\tau_{\boldsymbol{M}}^* T^* \boldsymbol{M}) = \tau_{\boldsymbol{M}}^* \det(T^* \boldsymbol{M}) = \tau_{\boldsymbol{M}}^* \Lambda^n T^* \boldsymbol{M},$$

where *n* is the dimension of M. Since M is orientable, it admits a natural metalinear structure that allows us to construct the bundle $N_{P}^{1/2}$ of half-forms normal to P which is a square root of the canonical bundle; i.e. $N_{P}^{1/2} = \sqrt{\tau_{M}^{*}\Lambda^{n}T^{*}M} = \tau_{M}^{*}\sqrt{\Lambda^{n}T^{*}M}$. The Lie derivative of forms induces on the canonical bundle K_{P} a partial covariant derivative ∇ defined along P. This, in turn, induces on $N_{P}^{1/2}$ a natural partial covariant derivative $\nabla^{1/2}$ defined along P. Therefore we can endow the line bundle $\bar{Q}^{\uparrow} \otimes N_{P}^{1/2}$ with the tensor product partial covariant derivative $\nabla' = \nabla[\bar{\mathbf{q}}^{\uparrow}] \otimes 1 + 1 \otimes \nabla^{1/2}$ defined along P. The space of P-polarized sections of the line bundle $\bar{Q}^{\uparrow} \otimes N_{P}^{1/2}$ is

$$\Gamma_{\boldsymbol{P}}(\bar{\boldsymbol{Q}}^{\uparrow} \otimes N_{\boldsymbol{P}}^{1/2}) = \{\xi \in \Gamma(T\boldsymbol{M}, \bar{\boldsymbol{Q}}^{\uparrow} \otimes N_{\boldsymbol{P}}^{1/2}) \colon \nabla_{V}^{\prime} \xi = 0, \ \forall \ V \in \Gamma(T\boldsymbol{M}, \boldsymbol{P}) \}.$$

The Hilbert space of GQ quantum states is given by the L^2 -completion of $\Gamma_{\boldsymbol{P}}(\bar{\boldsymbol{Q}}^{\uparrow} \otimes N_{\boldsymbol{P}}^{1/2})$. Since the line bundle $\bar{\boldsymbol{Q}}^{\uparrow} \otimes N_{\boldsymbol{P}}^{1/2} = \tau_{\boldsymbol{M}}^*(\bar{\boldsymbol{Q}} \otimes \sqrt{\Lambda^n T^* \boldsymbol{M}}) \to T\boldsymbol{M}$ is a pullback, its space of global sections is given by

$$\Gamma(T\boldsymbol{M}, \bar{\boldsymbol{Q}}^{\uparrow} \otimes N_{\boldsymbol{P}}^{1/2}) = C^{\infty}(T\boldsymbol{M}) \otimes_{C^{\infty}(\boldsymbol{M})} \Gamma(\boldsymbol{M}, \bar{\boldsymbol{Q}} \otimes \sqrt{\Lambda^{n} T^{*} \boldsymbol{M}}).$$

Taking into account now that the partial covariant derivative ∇' is also a pullback, we immediately obtain the identification

$$\Gamma_{\boldsymbol{P}}(T\boldsymbol{M}, \bar{\boldsymbol{Q}}^{\uparrow} \otimes N_{\boldsymbol{P}}^{1/2}) = \Gamma(\boldsymbol{M}, \bar{\boldsymbol{Q}} \otimes \sqrt{\Lambda^n T^* \boldsymbol{M}}).$$

The quantum operators on half-forms corresponding with position and momentum observables are just the same as (34); compare it with eq. 7.82, p. 128 of [28]. The difference between CQM and GQ lies in the way how the energy is quantized.

Concerning the energy \mathcal{H}_0 , from (33) we have the expression

(37)
$$\hat{\mathcal{H}}_{0}(\Psi^{\eta}) = \left(-\frac{1}{2}\overset{o}{\Delta}_{0} - A_{0} - \frac{1}{2}kf^{0}r_{0}\right)\Psi^{\eta},$$

and we can use (24) in order to write the first summand as $-\frac{1}{2}\overset{o}{\Delta}\Psi_0 \otimes \sqrt{\eta}$. In this way we realize that the only difference between the above formula and the corresponding formulae 7.114 on p. 134 (F = 0) and 10.59 on p. 180 ($F \neq 0$) of [28] is the factor in front of the scalar curvature r^2 .

In order to decide which factor must be used for introducing the scalar curvature in the energy operator we recall that in GQ the quantum operator corresponding to the kinetic energy is obtained by the Blattner-Kostant-Sternberg (BKS) method. This method is useful for those observables f, like energy, whose Hamiltonian vector field X_f does not preserve the polarization. The value of the corresponding quantum operator on a wave function Ψ is obtained by dragging Ψ using the flow of the lift of X_f to the half-form bundle and then projecting the result back to the space of polarized sections. Following [28, eq. 10.52], the computation of the energy operator by the BKS method yields at the pole of a normal coordinate system (where $\partial_i g_{jk} = 0$)

(38)
$$\mathcal{Q}(\psi^{\eta}b\otimes\sqrt{v}) = \overset{\circ}{\Delta}(\psi^{\eta}b)\otimes\sqrt{v}$$

We stress that here \sqrt{v} is just a local basis of the bundle of volume forms, and not the global section $\sqrt{\eta}$ (see (17) and the sentences thereafter). Then a computation at the pole of a normal coordinate system shows that

(39)
$$\overset{o}{\Delta}(\psi^{\eta}b) \otimes \sqrt{v} = (\overset{o}{\Delta}(\Psi) + \frac{1}{6}r\Psi)\sqrt{\eta}$$

(see also [36]). The right-hand side of the above formula is a globally defined tensor, while it is not possible to interpret the left-hand side as an intrinsic expression by means of the available connections.

3.1 Lemma. The following equality holds:

$$\overset{o}{\Delta}(\psi^{\eta}b)\otimes\sqrt{v}=\overset{o}{\Delta}(\Psi^{\eta})-2\bar{G}(\check{\nabla}^{o}(\psi^{\eta}b)\otimes\check{\nabla}^{o}\sqrt{v})-\psi^{\eta}b\otimes\bar{G}(\check{\nabla}^{o}\check{\nabla}^{o}\sqrt{v})$$

²The difference in sign is due to the fact that, like in [37], we use the opposite convention about the value of r with respect to [28]

$$\begin{array}{ll} (40) & \stackrel{o}{\Delta}(\Psi^{\eta}) = \bar{G}(\check{\nabla}^{o}\check{\nabla}^{o}(\psi^{\eta}b\otimes\sqrt{v})) \\ (41) & = \bar{G}(\check{\nabla}^{o}\check{\nabla}^{o}(\psi^{\eta}b))\otimes\sqrt{v} + 2\bar{G}(\check{\nabla}^{o}(\psi^{\eta}b)\otimes\check{\nabla}^{o}\sqrt{v}) + \psi^{\eta}b\otimes\bar{G}(\check{\nabla}^{o}\check{\nabla}^{o}\sqrt{v}), \end{array}$$

and the statement is proved by observing that

$$\overset{o}{\Delta}(\psi^{\eta}b)\otimes\sqrt{v}=\bar{G}(\check{\nabla}^{o}\check{\nabla}^{o}(\psi^{\eta}b))\otimes\sqrt{v}.$$

3.2 Theorem. At the pole of a normal coordinate system we have

$$\overset{o}{\Delta}(\Psi^{\eta}) = \overset{o}{\Delta}(\psi^{\eta}b) \otimes \sqrt{v} - \frac{1}{6}r\Psi^{\eta}.$$

Proof. Using the above Lemma we have

$$(42) \qquad \begin{array}{l} \overset{o}{\Delta}(\Psi^{\eta}) = \overset{o}{\Delta}(\psi^{\eta}b) \otimes \sqrt{v} + G^{ij}(\check{\nabla}^{o}_{i}(\psi b)\sqrt[4]{|g|} \otimes \Gamma^{h}_{jh}\sqrt{v}) + G^{ij}\psi b\partial_{i}\sqrt[4]{|g|} \otimes \Gamma^{h}_{jh}\sqrt{v} \\ + \psi^{\eta}b \otimes G(\check{\nabla}^{o}(\frac{1}{2}\Gamma^{h}_{ih}\check{d}^{i} \otimes \sqrt{v})) \\ = \overset{o}{\Delta}(\psi^{\eta}b) \otimes \sqrt{v} + G^{ij}(\check{\nabla}^{o}_{i}(\psi b)\sqrt[4]{|g|} \otimes \Gamma^{h}_{jh}\sqrt{v}) \\ + \frac{1}{2}\psi^{\eta}b \otimes G^{ij}(\partial_{i}\Gamma^{h}_{jh} + \Gamma^{k}_{ij}\Gamma^{h}_{kh} - \frac{1}{2}\Gamma^{k}_{ik}\Gamma^{h}_{jh})\sqrt{v})) \end{array}$$

At the pole of the normal coordinate system we have $\Gamma^i_{jk} = 0$, hence

(44)
$$\overset{o}{\Delta}(\Psi^{\eta}) = \overset{o}{\Delta}(\psi^{\eta}b) \otimes \sqrt{v} + \frac{1}{2}\psi^{\eta}b \otimes G^{ij}\partial_{i}\Gamma^{h}_{jh}\sqrt{v};$$

it can be proved that $r = \frac{3}{2}G^{ik}g^{pq}\partial_i\partial_kg_{pq}$ and that $\frac{1}{2}G^{ij}\partial_i\Gamma^h_{jh} = -\frac{1}{4}G^{ij}g^{hk}\partial_i\partial_jg_{hk}$, so that the statement is proved.

So, if, according to CQM, we define the energy operator using the Bochner Laplacian which takes into account the Riemannian connection on the square root bundle $\sqrt{\wedge^3 T^* M} \rightarrow M$ then the scalar curvature term which arises in GQ is canceled by a similar term arising from the covariant derivative of the base of sections of the square root bundle.

On the other hand, while the 'intermediate' term $\overset{o}{\Delta}(\psi^{\eta}b) \otimes \sqrt{v}$ obtained by the BKS method has no intrinsic meaning, the final result (*i.e.* the right-hand side of (39)) is intrinsic. CQM allows us to recover this term by adding a term with the scalar curvature multiplied by an arbitrary coefficient, using our quantum Lagrangian approach. So we can, in a sense, recover the expression of [28] through CQM.

4 Conclusions

We have discussed the two ways for defining the quantum energy operator proposed by CQM and GQ. The energy operators obtained by these two methods differ by a multiplication operator by a constant times the scalar curvature. This constant can be arbitrarily modified if one uses the Lagrangian approach, or even completely removed if one uses covariant derivatives of half-forms.

It is a well-known feature of GQ that non-trivial examples are very few since it is very easy to run into topological obstructions and several other complications. In all known examples of GQ whose spectral problem for the energy operator has been analyzed, the scalar curvature term is just zero or a constant. Among the latter ones we can mention the results obtained for the Landau problem on Riemann surfaces [19, 29, 20, 32, 33] and for the rigid body [30, 31]. In these cases the spectrum of the Schrödinger operator is modified by an overall shift.

At the moment, we can only say that the possibility that the scalar curvature plays no rôle in quantum mechanics is not remote. One possibility is that one might be able to modify the BKS method in such a way as to incorporate the action of the Riemannian connection on the square root bundle. In general, most well known polarizations are endowed with a fibre metric and therefore in principle it should be possible to define a Riemannian connection acting on half-forms. Another possibility is that the whole BKS procedure could be re-expressed in an 'infinitesimal' way through the parallel transport of the connection χ on the infinite-dimensional bundle. It is known [6, 7, 8] that such a parallel transport leads to the Feynman integral formulation, and this could also be useful in order to perform a covariant analysis of De Witt's approach [4].

We hope to solve the problem of scalar curvature in quantum mechanics in a future research.

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