Tautological Tuning of the Kostant-Souriau Quantization Map with Differential Geometric Structures

T. McClain *

Abstract

For decades, mathematical physicists have searched for a coordinate independent quantization procedure to replace the ad hoc process of canonical quantization. This effort has largely coalesced into two distinct research programs: geometric quantization and deformation quantization. Though both of these programs can claim numerous successes, neither has found mainstream acceptance within the more experimentally minded quantum physics community, owing both to their mathematical complexities and their practical failures as empirical models. This paper introduces an alternative approach to coordinate-independent quantization called tautologically tuned quantization. This approach uses only differential geometric structures from symplectic and Riemannian geometry, especially the tautological one form and vector field (hence the name). In its focus on physically important functions, tautologically tuned quantization hews much more closely to the ad hoc approach of canonical quantization than either traditional geometric quantization or deformation quantization and thereby avoid some of the mathematical challenges faced by those methods. Given its focus on standard differential geometric structures, tautologically tuned quantization is also a better candidate than either traditional geometric or deformation quantization for application to covariant Hamiltonian field theories, and therefore may pave the way for the geometric quantization of classical fields.

Keywords: Differential Geometric Methods in Theoretical Physics, Frontiers in Mathematical Physics, Geometrical Methods in Mathematical Physics, Non-relativistic Quantum Mechanics

*Department of Physics and Engineering, Washington and Lee University, Lexington, VA 24450 USA, email: mcclaint@wlu.edu
1 Introduction

Though physically quite successful, canonical quantization is not a coordinate-independent mathematical process. Given two different coordinate systems $X = \{q^i, p_i\}$ and $Y = \{Q^i, P_i\}$ and the ordinary canonical quantization map $QC : \{q^i, p_i\} \mapsto \{q^i, -i\hbar \frac{\partial}{\partial q^i}\}$, the following diagram does not commute:

\[
\begin{array}{ccc}
\{q^i, p_i\} & \xrightarrow{QC} & \{q^i, -i\hbar \frac{\partial}{\partial q^i}\} \\
\downarrow Y & & \downarrow Y \\
\{Q^i, P_i\} & \xrightarrow{QC} & \{Q^i, -i\hbar \frac{\partial}{\partial Q^i}\}
\end{array}
\]

Intuitively, this means that the result of the quantization process depends explicitly on the coordinate system in which the canonical quantization process is carried out.

This is by no means a new observation, and there have been decades of research into how best to solve the problem. The first attempts were really just efforts to patch up the canonical quantization procedure by the addition of more ad hoc rules; see [1] for perhaps the most famous and enduring of these. This line of research has continued all the way to the present day (see, for example, [2] and [3]), and in fact remains more-or-less standard among experimentally minded quantum physicists. New discoveries of fundamental significance are still being made along these lines; see, for instance, [4].

However, among more mathematically minded quantum physicists (and, of course, among mathematicians) this ad hoc approach was long ago superseded by two quite different approaches. These two research programs are devoted to solving the basic problem that the procedure is canonical quantization – though physically very successful when implemented by sophisticated practitioners – is nevertheless mathematically ill defined. The first is geometric quantization, really begun by van Hove in the 1940s, but taken in its modern direction by Souriau and Kostant (among others) in the 1960s and 70s; see [5] and [6]. The second is deformation quantization, also really begun by van Hove, but given its modern form by Kontsevich (among others); see [7]. Both research programs can claim some major successes: mostly mathematical in the case of deformation quantization, both mathematical and physical in the case of geometric quantization. Researchers continue to produce new results of fundamental interest in geometric [8] [9] and deformation [10] [11] quantization, as well as to find new applications of the mathematical techniques of each program (see, for example, [12] and [13]).

However, both programs must contend with a basic problem in quantization: the theorems of Groenewald [14] and Van Hove [15] (among others; see, for
example, [16]) make it clear that no quantization map can satisfy all the requirements one might reasonably hope to impose upon it for all possible functions on phase space. The goal of this paper is to introduce an approach to quantization that starts from the same point as geometric quantization but proceeds in a rather different manner, using only standard symplectic and differential geometric structures of the base and phase space manifolds to produce the quantization map. In light of the Groenewald-Van Hove theorems, no effort is made to make sure that the quantization map “works” for all possible functions on phase space. Instead, this approach assumes that the map only needs to quantize a tiny handful of important phase space functions. More will be said about the merits and demerits of this approach in the conclusion.

2 Symplectic Structures for Quantization

The material in this section is standard and can be found in any textbook on geometric Hamiltonian mechanics or symplectic geometry (see, for example, [17]). Readers already familiar with symplectic geometry can safely skip this section, as every effort has been made to make sure that it aligns with the notational conventions most common in the field. For readers at the opposite end of the spectrum, a certain amount of differential topology is necessary to understand symplectic geometry. The necessary material concerning differential manifolds, tangent spaces, differential forms, etc. can be found in any textbook on differential topology, as well as a good many textbooks on geometric methods in physics (see, for example, [18]).

Let the differentiable manifold \( Q \) represent the space in which our particle or particles are able to move. In the most common case, this is simply three-dimensional space \( Q = \mathbb{R}^3 \). The phase space for the particle is then

\[
P = T^*Q
\]

with projection map \( \pi : P \to Q \). It is this space upon which all the geometric structure of the theory will be built. The fundamental element of the symplectic structures of this space is the tautological (or canonical, or many other names) one-form, \( \theta \). It lives not on \( P \) but on the cotangent space \( T^*P \), and it is defined intrinsically by

\[
\theta_p(v) = p \circ \pi_* v
\]

where \( v \in T_pP \) is any vector in the tangent space \( TP \) over the point \( p \), \( \pi_* : TP \to TQ \) is the differential of the projection map \( \pi \), and \( p \in P \) is any point in \( P \). In terms of local coordinates \( \{ q^i, p_i \} \) on \( P \), one can write \( v \in T_pP = v^i \frac{\partial}{\partial q^i} + v_i \frac{\partial}{\partial p_i} \), \( \pi_* = \frac{\partial}{\partial q^i} \otimes dq^i \), and \( p = p_i dq^i + q^i e_i \) so that \( \theta_p(v) = v^i p_i \). In other words, \( \theta \) is a one-form on \( T^*P \) that can be written in coordinates as

\[
\theta = p_i dq^i
\]
Though the typical use of the tautological one-form $\theta$ is simply to produce the symplectic form $\omega$, this approach will make more use of it than is standard. Indeed, it is the word tautological from the name tautological one-form that gives rise to the name tautologically tuned quantization, for reasons that should be clear by the end of the next section.

Continuing the story of the standard symplectic structures, the single most important symplectic structure in the standard approach is undoubtedly the symplectic form $\omega$, the exterior derivative of the tautological one-form

$$
\omega = d\theta = dp_i \wedge dq^i
$$

where the second equality holds in (and indeed defines) canonical coordinates on the manifold $P$. In the case that $M = \mathbb{R}^3$, this reads (for those unfamiliar with the Einstein summation convention and/or wedge product)

$$
\omega = dp_1 \otimes dq^1 + dp_2 \otimes dq^2 + dp_3 \otimes dq^3 - dq^1 \otimes dp_1 - dq^2 \otimes dp_2 - dq^3 \otimes dp_3
$$

Since the symplectic form is non-degenerate (meaning that $\omega(u, v) = 0 \quad \forall \quad v \iff u = 0$), it is possible to associate with each function $f \in C^\infty(M)$ a vector field $X_f \in X(M)$ (usually called the Hamiltonian vector field of $f$) via

$$
\omega(X_f, -) = df
$$

In coordinates, this amounts to the assignment

$$
X_f = -\frac{\partial f}{\partial p_i} \frac{\partial}{\partial q^i} + \frac{\partial f}{\partial q^i} \frac{\partial}{\partial p^i}
$$

This assignment, in turn, make it possible to define a Poisson structure $\Pi$, with the defining property that

$$
\Pi(df, dg) = [X_f, X_g]
$$

for all $f, g \in C^\infty(M)$, where the bracket $[X_f, X_g] = X_f X_g - X_g X_f$ is the ordinary commutator of two vector fields. In canonical coordinates, this definition of $\Pi$ gives us

$$
\Pi = \frac{\partial}{\partial q^i} \wedge \frac{\partial}{\partial p_i}
$$

Finally, it is necessary to define a less standard symplectic structure, namely the vector field that results from contracting the Poisson structure $\Pi$ and the tautological one-form $\theta$. One might call this the tautological vector field. Though it is not the Hamiltonian vector field of any function $f$, it is essential in tautologically tuned quantization. In analogy with the Hamiltonian vector fields, it will be called $X_\theta$. The operations mentioned above give us

$$
X_\theta = \Pi(\theta) = p_i \frac{\partial}{\partial p_i}
$$

where the second equality once again holds in canonical coordinates on $P$. 
3 Tautologically Tuned Quantization

3.1 The Kostant-Souriau quantization map

There exists a simple quantization scheme that uses only the symplectic structures of the previous section to produce a map from smooth functions on the phase space $P$ to linear operators on (complex) phase space functions. This map – first introduced by Kostant and Souriau in the 1970s in [1] – is given by

$$Q_{KS}(f) := f - X_f \theta + i\hbar X_f = f - p_i \frac{\partial f}{\partial p_i} + i\hbar \frac{\partial f}{\partial q_i} \frac{\partial}{\partial p_i} - i\hbar \frac{\partial f}{\partial q_i} \frac{\partial}{\partial q_i} \tag{11}$$

Though relatively straightforward to define, this quantization map has many very nice properties. For instance, it maps the canonical coordinate functions to (mostly) appropriate looking operators:

$$Q_{KS}(q^i) = q^i + i\hbar \frac{\partial}{\partial p_i} \tag{12}$$

(but note the strange looking momentum coordinate derivative) and

$$Q_{KS}(p_i) = -i\hbar \frac{\partial}{\partial q_i} \tag{13}$$

It even maps the angular momentum function $L_3$ (as well as the other two) to a (mostly) appropriate looking operator:

$$Q_{KS}(L_3) = Q_{KS}(q^1 p_2 - q^2 p_1) = i\hbar (p_2 \frac{\partial}{\partial p_1} - p_1 \frac{\partial}{\partial p_2} - q^1 \frac{\partial}{\partial q^2} + q^2 \frac{\partial}{\partial q^1}) \tag{14}$$

The presence of the momentum coordinate derivatives in these operators is embarrassing, but if these could be eliminated then the operators look pretty good. However, it is easy to see that this map is far from perfect. For example, the one dimensional simple harmonic oscillator Hamiltonian maps to

$$Q_{KS}(H_{SHO}) = Q_{KS}\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2\right) = i\hbar (\frac{p}{m} \frac{\partial}{\partial q} + m\omega^2 q \frac{\partial}{\partial p}) - \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \tag{15}$$

which is a far cry from the expected

$$Q(H_{SHO}) = -\hbar^2 \frac{\partial^2}{\partial q^2} + \frac{1}{2}m\omega^2 q^2 \tag{16}$$

of canonical quantization (and correct physics).

Solving this problem will be the main focus of the last part of this section. But first it is necessary to more carefully define the space upon which these operators will act.
3.2 The space of quantum states

As part of solving the problem that the Kostant-Souriau quantization map produces operators with both position coordinate and momentum coordinate derivatives, it is necessary to look more closely at the space of quantum states. Those familiar with quantum theory will quickly recognize that complex-valued functions on phase space have too many independent variables to be genuine wave functions: in the position representation, wave functions depend upon the position coordinates and in the momentum representation they depend upon the momentum coordinates, but in no case do they depend upon both. It is easy to eliminate this problem by requiring that wave functions representing genuine quantum states be polarized (in the language of differential geometry). Given the symplectic structures defined thus far, the most natural polarization to choose is the vertical one. Define a vertical vector in the tangent space $T_P P$ as one for which

$$\pi^*(v) = 0$$

where $\pi^*$ is once again the differential of the projection map $\pi : P \to Q$ used in (3). In local canonical coordinates, these vertical vectors have the form $v = v_i \frac{\partial}{\partial p_i} + 0 \frac{\partial}{\partial q_i}$. A vector field is called vertical if it is vertical over every point in $P$, and $V(P)$ is defined to be the space of all vertical vector fields in $X(P)$. With this notion of vertical vectors it is possible to identify the space of quantum states $S$ as

$$S = \{ \Psi \in C^\infty(P, \mathbb{C}) | v \Psi = 0 \ \forall \ v \in V P \}$$

In local canonical coordinates genuine wave functions must have the form $\Psi(q^i, p_i) = \Psi(q^i)$. This restriction means that the momentum coordinate derivatives in the operators of the (3.1) are nilpotent when acting on wave functions. This almost – but not quite – removes the first difficulty of the previous section. The remaining issue is that the momentum coordinate derivatives are not necessarily nilpotent when acting on other operators, as in a commutator or any other instance in which two or more operators are applied in succession. The existence of these momentum derivatives seems guaranteed whenever a quantization map is generated solely from symplectic structures.

It is worth considering a new problem created by declaring wave functions to be polarized functions over $P$: there is no longer a good norm on this space. If the space under consideration were still the full space of functions over $P$, it would have been possible to use the natural volume form on $P$ defined by the symplectic structure to define a norm on this function space. As a brief reminder, the natural volume form on $P$ is

$$\text{vol}_P := \frac{1}{n!} \wedge^n \omega = dq^1 \wedge ... \wedge dq^n \wedge dp_1 \wedge ... \wedge dp_n$$

where $n$ is the dimension of the base space $Q$ (that is, $n = \frac{1}{2} \dim P$), $\omega$ is the symplectic form of (4), the notation $\wedge^n \omega$ means to take the exterior product of $\omega$.
with itself $n$ times, and the second equality holds in local canonical coordinates. The natural norm on $C^\infty(P, C)$ is then:

$$\langle \Psi, \Phi \rangle := \int_P \Psi^* \Phi \ dvol_P \quad (20)$$

The problem now is that this norm is always undefined for the polarized functions of (18). Taking canonical coordinates in which $\Psi$ and $\Phi$ are functions of the $q^i$ alone gives

$$\langle \Psi, \Phi \rangle := \int_P \Psi^* \Phi \ dq_1 \wedge ... \wedge dp_n = \int \Psi^* \Phi \ dq_1 \wedge ... \wedge dq^n \times \int dp_1 \wedge ... \wedge dp_n$$

Though the first integral may be finite for appropriate functions $\Psi$ and $\Phi$, the second never is.

It is noteworthy that there exists a straightforward (though typically unmentioned) solution to this problem, albeit one that only works with the vertical polarization defined above. Since tautological tuning works solely with the vertical polarization, this solution is worth presenting here. With this restriction, the norm problem can be solved by introducing a Riemannian metric on $Q$, which in turn induces a natural volume form on $Q$. This volume form can then be pulled back to produce an integration measure on $P$, such that

$$\langle \Psi, \Phi \rangle := \int_P \pi^*(\psi^* \phi) \ \pi^* dvol_Q = \int_Q \psi^* \phi \ dvol_Q \quad (21)$$

This is now finite for appropriate wave functions $\psi$ and $\phi$. The introduction of a metric on $Q$ will pay dividends later, too; see (??) and below. On the other hand, creating a viable norm on $P$ has required the introduction of an arbitrary Riemannian metric on $Q$, which is another piece of data that must be supplied to create a viable theory.

### 3.3 Tautologically tuned quantization

It is now possible to remove the difficulty with quadratic Hamiltonians of section 3.1 in a very unusual (compared to geometric quantization) way. The resulting quantization map is well-defined, uses only symplectic structures from Section 2 and standard structures from Riemannian geometry, and is coordinate independent. It is, however, also rather “unnatural” looking as a result of its having been tuned to quantize specific functions. More will be said about this concern in the last section.
As a first step, define a tautologically tuned quantization map $Q_{TT1}$:

$$Q_{TT1}(f) = f + \lim_{\epsilon \to 0} \frac{X_\theta f}{X_\theta f + \epsilon} (i\hbar X_f - X_\theta f)$$

$$= f + \lim_{\epsilon \to 0} \frac{p_i \frac{\partial f}{\partial p_i}}{p_i \frac{\partial f}{\partial p_i} + \epsilon} \left( i\hbar \frac{\partial f}{\partial q^i} \frac{\partial}{\partial p_i} - i\hbar \frac{\partial f}{\partial p_i} \frac{\partial}{\partial q^i} - p_i \frac{\partial f}{\partial p_i} \right)$$  \hspace{1cm} (22)

where the second equality holds in local canonical coordinates. This map is called “tautologically tuned” because it uses the tautological vector field $X_\theta$ to try to eliminate the extraneous momentum derivatives in the resulting operators. Intuitively, the map is being amended (in a geometrically invariant way) to take into account the specific function $f$ being quantized.

This map is at least partially successful at removing the momentum derivatives, as in local canonical coordinates it gives:

$$Q_{TT1}(q^i) = q^i$$ \hspace{1cm} (23)

(note the elimination of the momentum coordinate derivative) and

$$Q_{TT1}(p_i) = -i\hbar \frac{\partial}{\partial q^i}$$ \hspace{1cm} (24)

but still

$$Q_{TT1}(L^3) = Q_{TT1}(q^1 p_2 - q^2 p_1) = i\hbar \left( p_2 \frac{\partial}{\partial p_1} - p_1 \frac{\partial}{\partial p_2} - q^1 \frac{\partial}{\partial q^2} + q^2 \frac{\partial}{\partial q^1} \right)$$ \hspace{1cm} (25)

where the extraneous momentum derivatives have survived despite the tuning process.

Moreover, this first attempt at tautological tuning does nothing to solve the problem with the simple harmonic oscillator Hamiltonian (nor other Hamiltonians quadratic in the momenta):

$$Q_{TT1}(H_{SHO}) = Q_{TT1}(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2) = i\hbar (-\frac{p}{m} \frac{\partial}{\partial q} + m\omega^2 q \frac{\partial}{\partial p}) - \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$$ \hspace{1cm} (26)

This fundamental problem with quadratic Hamiltonians can be solved by adding a second tuned contribution to the quantization map, provided there exists a Riemannian metric on $P$. Unfortunately, it will have no impact on the problem of extraneous momentum derivatives. It is then possible to define a second tautologically tuned quantization map $Q_{TT2}$.
\[ Q_{TT2}(f) := f + \lim_{\epsilon \to 0} \frac{2X_\theta f - X_\theta^2 f}{2X_\theta f - X_\theta^2 f + \epsilon} (i\hbar X_f - X_\theta f) \]
\[ + \frac{1}{2} \lim_{\epsilon \to 0} \frac{X_\theta^2 f - X_\theta f}{X_\theta^2 f - X_\theta f + \epsilon} \left( -\frac{\hbar^2}{m} \Delta - X_\theta^2 f + X_\theta f \right) \]  

(27)

where \( \Delta \) is the geometr's Laplacian \( \Delta = \star d \star d \), and the Hodge dual \( \star \) is taken with respect to the (newly posited) Riemannian metric on \( P \). Some physicists worry that terms like \( X_\theta^2 \) are not coordinate invariant. This is not true. Skeptics are invited to explicitly check that the following diagram is indeed commutative for all coordinate transformations \( Y \):

\[
\begin{array}{c}
X_\theta \xrightarrow{\circ X_\theta} X_\theta^2 \\
\downarrow Y \quad \downarrow Y \\
X_\theta \xrightarrow{\circ X_\theta} X_\theta^2
\end{array}
\]

Tuning is much more prominent in this second map, but the outcome is the successful quantization of quadratic Hamiltonians. In local canonical coordinates, this second map gives:

\[ Q_{TT2}(q^i) = q^i \]  

(28)

and

\[ Q_{TT2}(p_i) = -i\hbar \frac{\partial}{\partial q^i} \]  

(29)

and

\[ Q_{TT2}(L^3) = Q_{TT1}(q^i p_2 - q^2 p_1) = i\hbar(p_2 \frac{\partial}{\partial p_1} - p_1 \frac{\partial}{\partial p_2} - q^1 \frac{\partial}{\partial q^2} + q^2 \frac{\partial}{\partial q^1}) \]  

(30)

(the extraneous momentum derivatives have again survived despite the tuning process) but now

\[ Q_{TT2}(H_{SHO}) = Q_{TT2}(\frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 q^2) = \frac{1}{2}m\omega^2 q^2 - \frac{\hbar^2}{2m} \Delta \]  

(31)

which is finally the expected result for the simple harmonic oscillator, albeit with extraneous momentum derivatives from \( \Delta \) that – though nilpotent on wave functions – may nonetheless be problematic upon composition with other operators (as in commutators).
Though the problems of the fundamentally incorrect quantization of quadratic Hamiltonians by (11) and the undefined norm of (20) have now been solved (albeit not without cost), nothing has really been done to solve the problem of extraneous momentum derivatives. It is important, though, to characterize exactly how bad this remaining problem really is. First, since the resulting operator will act only on vertically polarized wave functions, there is no problem when it comes to the action of these operators on wave functions: the extraneous momentum derivatives are nilpotent. The problem comes from the composition of operators with other operators. For example, in local canonical coordinates:

\[
\left[ Q_{TT2}(L^1), Q_{TT2}(L^2) \right] = \left[ Q_{TT2}(q^2p_3 - q^3p_2), Q_{TT2}(q^3p_1 - q^1p_3) \right]
\]

\[
= -\hbar^2 \left[ p_3 \frac{\partial}{\partial p_2} - p_2 \frac{\partial}{\partial p_3} - q^2 \frac{\partial}{\partial q^3} + q^3 \frac{\partial}{\partial q^2} \right] \left[ p_1 \frac{\partial}{\partial p_3} - p_3 \frac{\partial}{\partial p_1} - q^3 \frac{\partial}{\partial q^1} + q^1 \frac{\partial}{\partial q^3} \right]
\]

\[
= i\hbar Q_{TT2}(L^3) \quad (32)
\]

Similar calculations show that the extraneous momentum derivatives do not affect the commutation relations between any of the angular momentum operators.

What about the commutation relations between the angular momentum operators and a standard quadratic Hamiltonian? Taking the case of \( L^3 \) and the free particle Hamiltonian gives:

\[
\left[ Q_{TT2}(L^3), Q_{TT2}(H_{FP}) \right] = \left[ i\hbar \left( p_2 \frac{\partial}{\partial p_1} - p_1 \frac{\partial}{\partial p_2} - q^1 \frac{\partial}{\partial q^2} + q^2 \frac{\partial}{\partial q^1} \right), q^3 \right] = 0 \quad (33)
\]

Similar calculations show (naturally) that the free particle Hamiltonian also still commutes with the other angular momentum operators. Since the extraneous momentum operators are nilpotent when acting on all polarized functions \( f(p) = f(q^1) \), the commutation relations between the angular momentum operators and all quadratic Hamiltonians are preserved.

This analysis shows that the commutation relations are correct for the position, momentum, angular momentum, and (quadratic) Hamiltonian operators. From the perspective of physics, one might therefore conclude that the extraneous momentum operators are not such a very great problem after all.

4 Conclusion

The first and most obvious objection to the tautologically tuned quantization maps of the previous section is that they seem rather artificial. The second map,
in particular, seems only to be good for adding quadratic Hamiltonians to the list of correctly quantized functions, and it does so at the cost of considerable additional complexity.

This objection is completely warranted as far as it goes, but it is also totally unphysical. Physically, the phase space functions that need to be quantized are actually quite limited, corresponding (more-or-less) to the generators of important symmetry transformations. But these physically important functions on phase space are correctly quantized, at least in terms of their action on properly polarized wave functions: the position and momentum operators that generate boosts and spatial translations, the angular momentum operators that generate spatial rotations, and the (quadratic) Hamiltonian operators that generate time translations. Not only that, but their commutation relations are also correct. And all this has been achieved without ever resorting to the esoteric techniques of geometric quantization: no complex polarizations, no half-form quantization, etc.

It is would be better to have a rigorous way of defining which functions are necessary to quantize than to say that they should be “physically important.” But the hope is that this work has provided food for thought about alternative approaches to the quantization of particle systems.

Perhaps more importantly, because the tautological tuning process uses only symplectic and differential geometric structures that are present in both Hamiltonian particle systems and covariant Hamiltonian field systems, it seems much more likely to be extensible to the quantization of classical fields than traditional geometric quantization or deformation quantization have been. Indeed, some applications along these lines have already been tried, with mixed success [19]. This is a clear area for future research in tautologically tuned quantization.

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