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Posted Date: 14 April 2023

doi: [10.20944/preprints202302.0144.v2](https://doi.org/10.20944/preprints202302.0144.v2)

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## Article

# On Quantization, Contextuality & the Koopman-von Neumann Formulation

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**Abstract:** This article proposes a novel formulation of quantization, which considers the Koopman-von Neumann formulation (KvN) and ordinary non-relativistic quantum mechanics (OQM) as unitarily inequivalent representations of the same underlying structure. The approach is grounded in the notion that contextuality, rather than occurrence of Plank's constant, is the fundamental aspect of quantum mechanics. The motivation for this novel view arises from the limitations of traditional approaches to quantization, combined with previous research demonstrating contextuality in KvN. Using a representation-theoretic approach, both KvN and OQM are regarded as valid quantum theories, separated by a superselection rule.

**Keywords:** quantization; Koopman-von Neumann formulation; contextuality; classical statistical mechanics; reductionism; the classical limit

## 1. Introduction

The traditionally view of *quantization* (TQ) is as follows:

*Quantization is an algorithm for translating a classical theory into a corresponding quantum theory such that, as  $\hbar \rightarrow 0$ , the classical theory is re-obtained.* (TQ)

Thus, quantization, as traditionally understood, depends on the assumption that  $\hbar$  is fundamental to what constitutes quantum mechanics, and the limit  $\hbar \rightarrow 0$  is referred to as the "classical limit."  $\hbar$  being a constant of nature, the limit  $\hbar \rightarrow 0$  means that  $\hbar$  is small compared to other quantum numbers. In this sense, quantum mechanics is related to classical mechanics in the sense of physicist's reductionism [1]. This is the same way that Galilean relativity is derived from special relativity at velocities small enough compared to the speed of light, i.e. in the  $c \rightarrow \infty$  limit. Given this reductionist perspective, it is therefore easy to accept the traditional view of quantization, with  $\hbar$  being a crucial part of what constitutes quantum mechanics.

Even if ignoring the question of whether  $\hbar \rightarrow 0$  can be considered a properly defined mathematical limit [2,3], the reductionist view of what constitutes the essence of quantum mechanics is still plagued by a major problem. This problem is that  $\hbar$  is not inherent to the formalism of quantum mechanics.

In the modern account of quantum mechanics it is viewed as a purely probabilistic incorporating the concept of *contextuality*, i.e. an observables inherent dependence on the actual context of measurement. As an example of contextuality, consider the double-slit experiment. A measurement of  $A$ —determining which slit the electron passed through—necessarily involves closing one of the slits. If a flash appears on the fluorescent screen, the electron must have passed through the open slit. The act of closing one slit is part of what constitutes the measurement of  $A$ , and therefore the measurement is not realized in the context of both slits being open. This by itself does not mean that  $A$  has no meaning without an actual measurement being performed. Rather, it means that  $A$  is manifested in a specific way through measurement, and that the way in which it is manifested matters. The way that it matters is that it turns up as an actual observable phenomenon. This is the phenomenon of quantum interference.

In [4], Feynman showed that quantum interference can be viewed as a 'violation' of the formula of total probability as known from classical probability theory. He not only suggested that this is the

quantum phenomenon, but also that it is the sense in which the double-slit experiment is non-classical. That is, he claimed it to be 'non-classical' because it violates classical probability theory. In contrast, he noted that the formalism of quantum mechanics can account for the interference phenomenon. From this, he concluded that the formalism of quantum mechanics corresponds not only to a probability theory, but also to a 'non-classical' probability theory.

However, as Ballentine [5] and Koopman [6] have both correctly pointed out, there is no violation of the formula of total probability, as it is not expected to hold in the first place. Feynman overlooked the fact that in the double-slit experiment, three different measurement contexts were considered: first slit covered, second slit covered, and both open. Taking these into account, the formula of total probability is not expected to hold. The relevance of the different measurement contexts—contextuality—is not a violation of classical probability theory, but rather an inherent part of probability, as emphasized by Kolmogorov [7]. There is no 'classical' or 'non-classical' probability theory, only probability theory, and the formalism of quantum mechanics is in complete agreement with it.

**Remark 1.** *Note, this is not saying classical mechanics can account for the double-slit experiment. In fact, it cannot. It is just saying, that it does not violate 'classical' probability theory. So it is not 'non-classical' in the probabilistic sense.*

Feynman was, however, correct in his assessment of the significance of the 'violation' of the formula of total probability with regards to its relevance to quantum mechanics. In [8,9], within the framework of contextual probability theory, the 'violation' of the formula of total probability—more appropriately referred to as the **interference term**—is formalized as a measure of contextuality. In this formalism, when there is contextuality, it is manifested in the quantum formalism through the occurrence of non-commuting quantum observables.

**Remark 2.** *It should be clear from this that contextuality is not itself something inherently connected with the occurrence of  $\hbar$ . Hence there is neither from this perspective some inherent connection between the traditional view of quantization—statement (TQ)—and the modern probabilistic view of quantum mechanics.*

In the Schrödinger's cat thought experiment, it is with regards to contextuality that the supposed paradox appears: Consider the pure quantum state,

$$\psi := \frac{1}{\sqrt{2}} \left( |\text{alive}\rangle + \frac{e^{i\theta}}{\sqrt{2}} |\text{dead}\rangle \right), \quad (1)$$

and its corresponding mixed state,

$$D := \frac{1}{2} (|\text{alive}\rangle \langle \text{alive}| + |\text{dead}\rangle \langle \text{dead}|). \quad (2)$$

With regards to the 'dead/alive' observable, both states result in the same probability distribution for its potential outcomes. However, when considering a potential observable  $O$  that does not commute with the 'dead/alive' observable, these states result in differing probability distributions:

$$\begin{aligned} 0 &\neq |\langle o|\psi\rangle|^2 - \langle o|D|o\rangle \\ &= \frac{e^{-i\theta}}{2} \langle \text{dead}|o\rangle \langle o|\text{alive}\rangle + \frac{e^{i\theta}}{2} \langle \text{alive}|o\rangle \langle o|\text{dead}\rangle, \end{aligned} \quad (3)$$

where  $|o\rangle$  denotes an arbitrary eigenstate of  $O$ . This difference is exactly equal to the interference term. In the Schrödinger's cat thought experiment, the 'dead/alive' observable is manifested as the act of opening a box and checking if the cat is dead or alive. If there is a non-zero interference term, it would result in contextuality, meaning the 'dead/alive' observable would be context-dependent. This would

then mean that *death* would be inherently dependent on the manner in which it is checked. Therein lies the paradox.

**Remark 3.** Of course, quantum mechanics does not dictate that every observable property—such as *death*—corresponds to a quantum observable. The Schrödinger's cat thought experiment should therefore not be taken as an empirical statement, but rather as an illustration of the weirdness of contextuality, and perhaps as an argument that not all observables can be represented as quantum observables. This is a known issue in other areas of physics, for example, there can't be a superposition between states of different charges, as this would violate charge conservation. Rules prohibiting such superpositions are commonly referred to as superselection rules [10]. These will be discussed further in this article. It is possible that there are superselection rules in place preventing superpositions of the type in equation (1).

With Remark 3 in mind, it is nonetheless fruitful to consider an equivalent way in which contextuality could manifest in a Schrödinger's cat-type scenario through a unitary time-evolution. Imagine introducing a time-evolution operator of the form:

$$\hat{U}_t := e^{-iat} |\text{alive}\rangle \langle \text{alive}| + e^{-idt} |\text{dead}\rangle \langle \text{dead}|. \quad (4)$$

This form could be made sensible by assuming that the cat is not expected to die for the duration of interest, unless the radioactive isotope suddenly decays—i.e. a wave-function collapse occurs. With respect to this time-evolution, (1) transforms non-trivially, while (2) transforms trivially, offering a means of discerning a pure from a mixed state. This difference manifests as a difference in the interference term and hence corresponds to contextuality, as proven in more generality in the author's previous work [11]. Moreover, in [11], it was shown that classical statistical mechanics manifests contextuality in this sense.

This was done in [11] by reformulation classical statistical mechanics in the Hilbert space formalism of quantum mechanics in what is commonly known as the Koopman-von Neumann formulation [12–14]. We briefly present it here in terms of its more modern formulation [15]. Let  $U$  correspond to a Hamiltonian flow on a phase space  $\mathcal{P}$  associated with a Hamiltonian function  $H$ . We unitarily represent  $U$  on the Hilbert space  $L^2(\mathcal{P}, d\mu)$  as

$$\hat{U}_t \psi := \psi \circ U_{-t}, \quad (5)$$

where  $\mu$  is any  $U$ -invariant measure—e.g. such as  $dPdQ$ , with  $(P, Q)$  being canonical coordinates on  $\mathcal{P}$ . In contrast to ordinary non-relativistic quantum mechanics (OQM), in which the operators  $\hat{P}$  and  $\hat{Q}$  satisfy the canonical commutation relations (CCR),

$$[\hat{P}, \hat{Q}] = i\hbar, \quad (6)$$

the operators  $\hat{P}$  and  $\hat{Q}$  here instead commute. These are here instead defined as:

$$\begin{cases} (\hat{P}\psi)(\omega) := P(\omega)\psi(\omega) \\ (\hat{Q}\psi)(\omega) := Q(\omega)\psi(\omega) \end{cases} \quad (7)$$

for all  $\omega \in \hat{P}$ . According to the Born's rule, a state  $\psi_t \in L^2(\mathcal{P}, d\mu)$  gives rise to a probability distribution over phase space as  $|\psi_t|^2$ . Moreover, this distribution satisfies the (integrated) Liouville equation,

$$|\psi_{t+\Delta t}|^2 = |\psi_t|^2 \circ U_{\Delta t}, \quad (8)$$

The eigenstates  $|L\rangle$  of the Liouvillian,

$$\mathcal{L} := i \frac{d}{dt} \Big|_{t=0} \hat{U}_t, \quad (9)$$

hence correspond to thermodynamic equilibria, and consequently arbitrary superpositions of such,

$$c_L |L\rangle + c_{L'} |L'\rangle \quad (10)$$

correspond to non-equilibria, as they are not stationary in time. As a result, we find ourselves in a similar situation to the Schrödinger's cat scenario discussed earlier. In this scenario, the pure state described by equation (10) can be differentiated from its corresponding mixed state,

$$|c_L|^2 |L\rangle \langle L| + |c_{L'}|^2 |L'\rangle \langle L'|, \quad (11)$$

through the use of the unitary time evolution operator  $\hat{U}$ . This demonstrates contextuality in classical statistical mechanics.

Indeed, only in terms of the observables in KvN of the form  $F(\hat{P}, \hat{Q})$ , there is no contextuality [16]. The Liouvillian, however, is not an observable of this form. There is nothing inherent to KvN that prohibits the interpretation of the Liouvillian as an observable. For example, even if arguing in the style of algebraic quantum mechanics [17], such as the algebra  $C^\infty(\mathcal{P})$  subjected to the action,

$$f \in C^\infty(\mathcal{P}) \mapsto U \cdot f := f \circ U_{-t} \in C^\infty(\mathcal{P}), \quad (12)$$

of the time-evolution  $U$ , the Liouvillian is not part of this algebra—in corresponds to an outer rather than an inner automorphism of the algebra—but this does not exclude it as a potential observable. This means that the Liouvillian can only be an observable in representations  $\rho$  of this algebra if there also exists a representation  $\hat{\rho}$  of  $U$  such that

$$\rho(U \cdot f) = \hat{U}_t \rho(f) \hat{U}_{-t}, \quad (13)$$

which is exactly what KvN is. It does not mean that, in general, the Liouvillian cannot be an observable.

**Remark 4.** *In classical statistical mechanics, it is generally believed that states correspond to statistical ensembles, meaning that a gas described by a probability distribution in phase space is considered to be in a definite state at all times, represented by a point in phase space. Einstein believed that probability would play a similar role in quantum mechanics as it did in classical statistical mechanics, in the sense of being reducible to "incomplete knowledge" of the system's exact state [18]. However, the results of [11] suggest that this ensemble interpretation was never viable in classical statistical mechanics in the first place and hence remove the very reason for imposing it upon OQM. Instead, it suggests that the problem with the foundations of quantum mechanics lies with probability in general, to which contextuality is inherent. In line with this and [11], elsewhere it has also been shown that contextuality is relevant in classical statistics [19].*

It is the claim of this article that KvN is as 'quantum mechanical' as OQM. This has already been demonstrated in [11] to be the case in terms of contextuality. However, the traditional view of quantization—statement (TQ)—still offers a sense in which OQM is possibly more 'naturally connected' to Hamiltonian mechanics than KvN is, and hence could be a sense in which it could be considered as more 'quantum mechanical'. For instance, interpreting TQ in the sense of Dirac [20] as corresponding to 'turning brackets to commutators'—symbolically written as:

$$\{\cdot, \cdot\} \mapsto -\frac{i}{\hbar} [\cdot, \cdot], \quad (14)$$

where  $\{\cdot, \cdot\}$  denotes the Poisson bracket and  $[\cdot, \cdot]$  the operator commutator—offers such a 'natural connection' and distinguishes OQM over KvN. The issue with this 'Diracian approach' is what this symbolic relation (14) is supposed to correspond to mathematically. The well-known Groenewold-van Hove theorem [21–23] states:

**Theorem 1.** *Let  $\mathbb{P}$  denote the set of all polynomials in  $P$  and  $Q$  subjected to the Poisson bracket, and  $\mathbb{P}_k$  the sub-Lie algebra of polynomials of degree less than or equal to  $k \in \mathbb{N}$ . There is no irreducible representation  $\Lambda$  of  $\mathbb{P}_k$ , for  $k \geq 3$ , as self-adjoint operators on some Hilbert space such that*

$$\Lambda(\{\cdot, \cdot\}) = -\frac{i}{\hbar} [\Lambda(\cdot), \Lambda(\cdot)]. \quad (15)$$

In the proof of this theorem, it is shown that the well-known ordering ambiguity that arises in operators of the form  $F(\hat{P}, \hat{Q})$  due to the CCR is unavoidable, regardless of the ordering prescription applied. As a result, a mapping  $\Lambda$  fails to exist even for polynomials and certainly does not exist for the full Poisson algebra of smooth functions in phase space. Theorem 1 therefore implies that (14) cannot correspond to a unitary representation of the Poisson algebra of Hamiltonian mechanics.

A Groenewold-van Hove-type theorem will also be proven in Section 2 of this article. The proof of this theorem will also show that the ordering ambiguity is unavoidable, but this theorem rather focuses on it not being in the sense of Dirac that canonical quantization works. Despite this, canonical quantization is not disproven. Its empirical success cannot be denied. It is simply that the Diracian sense of *quantization* neither provides a 'proper' formulation of it nor provide a reason for its empirical success.

There are more advanced versions of *quantization* that aim to provide a proper formulation of canonical quantization and aligned with TQ, such as Deformation quantization [24,25] and Geometric quantization [26]. Of these, Deformation quantization is closer to the Diracian approach. Both of these approaches still work under the assumption that the Diracian approach is 'basically correct'. In the sense of the correct understanding of *quantization* only needing to drop one of the premises of the Groenewold-van Hove theorem:

- In Deformation quantization, the Poisson bracket is replaced by the Moyal bracket as the Lie algebraic structure of phase space. With respect to the Moyal bracket, the analogous mapping to  $\Lambda$  in Theorem 1 exists. As  $\hbar$  approaches zero, the Moyal bracket converges to the Poisson bracket on the phase space side. In this sense, deformation quantization is considered to be aligned with Theorem TQ.
- In Geometric quantization, the requirement for mapping  $\Lambda$  in Theorem 1 to be irreducible is dropped. The result as a 'too large' Hilbert space. In order to have agreement with canonical quantization, these extra degrees of freedom must be decoupled, which is achieved through a process referred to as 'polarization'.

The view of *quantization* presented here rejects TQ and the assumption that the Diracian view is 'basically correct'. The main reason for this rejection is that it is contextuality, not the presence of  $\hbar$ , that constitutes the essence of quantum mechanics. Additionally, TQ relies on a reductionist view of physics and science, which is plagued with more problems than commonly thought [27–30].

Mathematically, TQ manifests as the CCR, leading to the consideration of the Diracian view. However, as will be shown in Section 2, the CCR cannot be considered as the quantum analogue of  $\{P, Q\} = 1$ —i.e. as a way of preserving the notion of *canonical coordinates* in the formalism of quantum mechanics. This is because the Poisson bracket in Hamiltonian mechanics is invariant under the large symmetry group of canonical transformations, while OQM violates this symmetry. Others—such as Gukov and Witten [31]—have pointed out that canonical quantization depends on the choice of canonical coordinates in which it is performed. In this article, this dependence is not only taken as a reason to reject the Diracian view of quantization, but also as the defining characteristic

of *quantization*. In the view of *quantization* presented in Section 3, the breaking of general canonical coordinate invariance will be considered an inherent part of *quantization*.

This new view postulates that the relevant structures of Hamiltonian mechanics with regards to *quantization* are what will be referred to as 'flow structures'. A flow structure consists of a Hamiltonian flow, its inherent symmetry of canonical transformations and a choice of canonical coordinates. KvN and OQM will be shown to correspond to simply inequivalent representations of Flow structures, and therefore they have been made as 'quantum mechanical' not only in terms of both exhibiting contextuality, but also in terms of both resulting from quantization.

The structure of this article is as follows: In Section 2, the limitations of the Diracian view of *quantization* in properly formalizing canonical quantization are demonstrated. It is shown that breaking the invariance of the choice of canonical coordinates is a fundamental aspect of canonical quantization, and this is suggested as the underlying reason for the limitations of the Diracian view. In Section 3, a new approach to quantization is proposed, which reinterprets this fundamental aspect as a feature of quantization rather than a hindrance. Both KvN and OQM are shown to be valid outcomes of this new quantization. Finally, in Section 4, the results and conclusions of the article are summarized and clarified.

## 2. Flaws of the Conventional View of Quantization

In the introduction of this article, **TQ** was primarily was criticized on the basis of it adhering rather to the  $\hbar$ -notion of quantum mechanics, rather than the modern in terms of contextuality, and as it presupposes a reductionist view of physics. In this section two claims associated to **TQ** of a more purely mathematical nature will be scrutinized. These claims are:

**Claim 1.** *The CCR,*

$$-\frac{i}{\hbar} [\hat{P}, \hat{Q}] = I, \quad (16)$$

*is the quantum version of the relation*

$$\{P, Q\} = I, \quad (17)$$

*in Hamiltonian mechanics, which states that the coordinate chart  $(P, Q)$  is canonical. Hence allowing us to refer to the pair  $(\hat{P}, \hat{Q})$  as 'canonical' in a similar sense as  $(P, Q)$  is.*

and

**Claim 2.** *Quantization corresponds to 'turning brackets to commutators',*

$$\{\cdot, \cdot\} \mapsto -\frac{i}{\hbar} [\cdot, \cdot]. \quad (18)$$

*More formally interpreted as a unitary representation of a sub-Lie algebra of the Poisson algebra associated with Hamiltonian mechanics.*

Claim 1 suggests that there is an equivalent concept of *canonical coordinates* in the formalism of quantum mechanics. If Claim 2 were true in its strongest possible sense—if *quantization* corresponded to a unitary representation of the Poisson algebra associated with Hamiltonian mechanics—then it might be possible to infer (16) as an analogous condition to (17) as a condition for *canonical coordinance*. However, it has long been known that *quantization* does not correspond to a unitary representation of the Poisson algebra associated with Hamiltonian mechanics, as demonstrated by the Groenewold-van Hove theorem. Therefore, Claim 1 cannot be argued for in this manner. For the concept of an observable  $P$  being the canonical conjugate of an observable  $Q$  is deeper than its manifestation in (17) in terms of the Poisson bracket. It has its roots in the transition from the Lagrangian to the Hamiltonian formalism and the symmetry group of canonical transformations in the latter. The actual utility of the Poisson

structure lies in its invariance under this group. Therefore, in this context, Claim 1 will be dismissed by showing that canonical quantization violates the invariance of the choice of canonical coordinates—i.e. that canonical quantization explicitly depends on the choice of canonical coordinates in which it is performed.

In subsection 2.1, the structure of modern classical mechanics will be reviewed, highlighting the origin of the Poisson structure in relation to canonical transformations and the transformation from the Lagrangian to the Hamiltonian formulation of classical mechanics. In subsection 2.2, the explicit definition of canonical quantization will be presented and a counterexample will be provided to show that it violates the symmetry of canonical transformations, thus proving that claim 1 is incorrect. In the same subsection, claim 2 will also be directly addressed, demonstrating that canonical quantization cannot be a unitary representation of a sub-Lie algebra of the Poisson algebra of Hamiltonian mechanics.

### 2.1. The structure of modern classical mechanics

The structure of Hamiltonian mechanics is a generalization of Lagrangian mechanics through symplectic geometry, but it is often introduced in classical mechanics textbooks as being derived from Lagrangian mechanics through a Legendre transform. By highlighting this, it becomes evident that canonical quantization is not solely tied to Hamiltonian mechanics. It encompasses the transformation from Lagrangian to Hamiltonian mechanics and is performed in a specific class of canonical coordinates. Given these fundamental principles, it is unlikely that either Claims 1 or 2 hold. Instead, the breaking of canonical transformations is seen as a defining aspect of canonical quantization, which will be incorporated into the new view of *quantization* presented in Section 3.

#### 2.1.1. From Lagrangian to Hamiltonian mechanics

Lagrangian mechanics occurs on the tangent bundle  $\mathcal{T}\mathcal{M}$ , wherein a point  $(Q, \dot{Q}) \in \mathcal{T}\mathcal{M}$ ,  $\dot{Q}$  corresponds to spatial velocity and  $Q$  to spatial position. The dynamics is described by a Lagrangian function

$$L : \mathcal{T}\mathcal{M} \rightarrow \mathbb{R}, \quad (19)$$

from which—by means of the principle of least action—one obtains the corresponding equations of motion:

$$\frac{d}{dt} \left. \frac{\partial L}{\partial \dot{Q}} \right|_{(\gamma(t), \dot{\gamma}(t))} = \left. \frac{\partial L}{\partial Q} \right|_{(\gamma(t), \dot{\gamma}(t))}, \quad (20)$$

where

$$\gamma : \mathbb{R} \rightarrow \mathcal{M} \quad (21)$$

is the particle's spatial path, and  $\dot{\gamma}$  is the derivative of that path.

To transition to the formalism of Hamiltonian mechanics, one works instead on the cotangent bundle  $\mathcal{T}^*\mathcal{M}$ . For a point  $(P, Q) \in \mathcal{T}^*\mathcal{M}$ ,  $P$  corresponds to conjugate momentum and  $Q$  corresponds to spatial position. Conjugate momentum is defined in terms of the specific dynamics [32]—i.e., in terms of the particular Lagrangian—as

$$P := \frac{\partial L}{\partial \dot{Q}}. \quad (22)$$

In Hamiltonian mechanics, the dynamics are determined by the Hamiltonian

$$H : \mathcal{T}^*\mathcal{M} \rightarrow \mathbb{R}, \quad (23)$$

which is obtained through a Legendre transform:

$$H := P \cdot \dot{Q} - L. \quad (24)$$

The fact that  $H$ , as defined in (24), indeed satisfies (23) can be shown using (20). The Hamiltonian equations of motion can then be derived:

$$\begin{cases} \dot{P} = -\frac{\partial H}{\partial Q} \\ \dot{Q} = \frac{\partial H}{\partial P} \end{cases} . \quad (25)$$

Note that in making this transition from Lagrangian to Hamiltonian mechanics, we have chosen a particular set of coordinates  $(P, Q)$ .

The generic formulation of Hamiltonian mechanics is one in terms of symplectic geometry [26,33]. This can be seen by constructing the Poisson bracket on  $\mathcal{T}^*\mathcal{M}$  in terms of the coordinates  $(P, Q)$ . For that purpose, let  $C^\infty(\mathcal{T}^*\mathcal{M})$  be the set of smooth functions on  $\mathcal{T}^*\mathcal{M}$ .

**Definition 1.** *The Poisson bracket*

$$\{\cdot, \cdot\} : (F, G) \in C^\infty(\mathcal{T}^*\mathcal{M}) \times C^\infty(\mathcal{T}^*\mathcal{M}) \mapsto F, G \in C^\infty(\mathcal{T}^*\mathcal{M}) \quad (26)$$

is defined as

$$\{F, G\} := \frac{\partial F}{\partial P} \frac{\partial G}{\partial Q} - \frac{\partial F}{\partial Q} \frac{\partial G}{\partial P}. \quad (27)$$

$$(P, Q) \mapsto (P'(P, Q), Q'(P, Q))$$

The utility of the Poisson bracket is that it is associated with a 'canonical' symmetry, meaning that certain coordinate transformations leave it invariant. Let

$$(P, Q) \mapsto (P'(O, Q), Q'(P, Q)) \quad (28)$$

be an arbitrary coordinate transformation from the coordinates  $(P, Q)$  to  $(P', Q')$ . Let  $\{\cdot, \cdot\}'$  denote an alternative Poisson bracket, defined in an analogous way to the original one, but with respect to the coordinates  $(P', Q')$ .

**Definition 2.** *The coordinates  $(P', Q')$  are canonical coordinates and the coordinate transformation (28) is a canonical transformation if*

$$\{\cdot, \cdot\} = \{\cdot, \cdot\}'. \quad (29)$$

The following is a standard result [33]:

**Theorem 2.**  *$(P', Q')$  are canonical coordinates if and only if*

$$\{P', Q'\} = 1. \quad (30)$$

Now, Hamilton's equations of motion (25) may be written in terms of the Poisson bracket as

$$\begin{cases} \dot{P} = \{H, P\} \\ \dot{Q} = \{H, Q\} \end{cases} , \quad (31)$$

and for any canonical coordinates  $(P', Q')$  we have

$$\begin{cases} \dot{P}' = \{H, P'\} \\ \dot{Q}' = \{H, Q'\} \end{cases} . \quad (32)$$

We have thus found a specific sense of *coordinates*—namely, canonical coordinates—in which the equations of motion can be expressed in an invariant form.

### 2.1.2. The Lagrangian mechanics-independent formulation of Hamiltonian mechanics

Note that the property of being canonical coordinates is still with respect to the specific Lagrangian from which we constructed the Hamiltonian mechanical system. The construction of the Poisson bracket is still based on particular coordinates  $(P, Q)$ , or any point transformation [32] of them. Hamiltonian mechanics has not yet been formulated in a manner that is entirely independent of Lagrangian mechanics. To achieve this, we need to find a way of defining the Poisson bracket that is inherently coordinate-invariant. This is where symplectic geometry comes into play. Although we will not present it in full here—the reader can refer to [26,33] for that—we will briefly summarize the main ideas. The following key points and standard results in symplectic geometry are relevant for our purposes:

- A **symplectic manifold** is a differentiable manifold  $\mathcal{P}$  equipped with a closed, non-degenerate 2-form  $\omega$ , called the **symplectic form**.
- The symplectic form allows us to associate a vector field  $X_F$ , called the **Hamiltonian vector field**, to any function  $F \in C^\infty(\mathcal{P})$ .
- We can replace the definition of the Poisson bracket in Definition 1 with the following:

$$F, G := \omega(X_F, X_G), \quad (33)$$

for all  $F, G \in C^\infty(\mathcal{P})$ .

- Symplectic manifolds are always even-dimensional.
- Darboux's theorem states that we can always (locally) find coordinates in which the Poisson bracket defined by (33) takes the same form as in Definition 1. These coordinates, called **Darboux coordinates**, correspond to canonical coordinates in this generic formulation of Hamiltonian mechanics.
- The cotangent bundle, the structure on which we previously constructed the Lagrangian mechanics-dependent formulation of Hamiltonian mechanics, is a specific example of a symplectic manifold whose Poisson bracket defined by (33) is equivalent to the one defined in Definition 1.
- The dynamics of the system is described by a Hamiltonian flow,

$$U : t \in \mathbb{R} \mapsto U_t \in \text{Sympl}(\mathcal{P}), \quad (34)$$

where  $\text{Sympl}(\mathcal{P})$  is the group of symplectomorphisms on  $\mathcal{P}$ —i.e the diffeomorphisms that preserve the symplectic form.

### 2.2. Mischaracterizations of quantization

In this subsection, we will first define *canonical quantization*. Then, using the information presented in the previous subsection, we will first disprove Claim 1—the assertion that the CCR corresponds to a 'quantum version' of *canonical coordinate*—and then disprove Claim 2—the Diracian view that quantization corresponds to 'turning brackets into commutators'.

#### 2.2.1. Canonical quantization

In the typical treatment of canonical quantization, it is implicit in its usage but often not emphasized enough that the prescription is explicitly defined in terms of particular canonical coordinates  $(P, Q)$ . A notable exception to this is Gukov and Witten in [31], where it is also stated that canonical quantization is dependent on the particular choice of coordinates. Here, canonical quantization will be properly defined in this manner, making this potential coordinate dependence explicit. By performing canonical quantization with respect to another choice of canonical coordinates, it will be shown that this yields an inequivalent quantum theory, and hence that canonical quantization is indeed not implicitly independent of the choice of canonical coordinates.

**Definition 3.** Let  $(\mathcal{T}\mathcal{M}, L)$  be a classical mechanical system described in terms of Lagrangian mechanics with an associated Lagrangian  $L$ . To **canonically quantize** this system, we represent the observables  $P$  and  $Q$  as quantum observables  $\hat{P}$  and  $\hat{Q}$  on some Hilbert space  $\mathcal{H}$  such that their respective spectra match the range of possible values of their classical counterparts, i.e.,  $\mathbb{R}$ , and such that the CCR holds,

$$[\hat{P}, \hat{Q}] = i\hbar. \quad (35)$$

The generator of time evolution is set to be the operator

$$H(\hat{P}, \hat{Q}), \quad (36)$$

known as the **quantum Hamiltonian**, and is interpreted as the quantum observable of energy of the system.

Moreover, associated to this definition of *canonical quantization* is also the additional assumption that: Given a classical observable  $F$  on  $\mathcal{T}^*\mathcal{M}$ , its quantum counterpart is given by

$$F(\hat{P}, \hat{Q}), \quad (37)$$

which inherits its interpretation from the classical observable  $F$ . This is not only the case for the Hamiltonian  $H$ —as explicitly stated in (36)—but it also applies to other observables such as orbital angular momentum which take the form  $\hat{\mathbf{P}} \times \hat{\mathbf{Q}}$  [34]. However, it is important to note that there is the well-known issue of ordering ambiguities in the symbolic expressions (36) and more generally in (37). While this definition of canonical quantization is not mathematically rigorous due to this ordering ambiguity, it is sufficient enough for our purposes here. The main point is to emphasize that canonical quantization is defined with respect to a particular set of preferred canonical coordinates. For this purpose, we consider another set of canonical coordinates  $(P', Q')$ , which are related to the original coordinates  $(P, Q)$  through the transformation,

$$\begin{cases} P'(P, Q) \\ Q'(P, Q) \end{cases}. \quad (38)$$

If it were true that the choice of canonical coordinates did not matter in canonical quantization, then we should have

$$i\hbar = [P'(\hat{P}, \hat{Q}), Q'(\hat{P}, \hat{Q})]. \quad (39)$$

To show that this is not the case, we consider the simple harmonic oscillator, whose Hamiltonian is given by

$$H_{\text{osc}}(P, Q) = \frac{1}{2}P^2 + \frac{1}{2}Q^2. \quad (40)$$

We perform a canonical transformation to the action-angle coordinates  $(\Theta, E)$ , where

$$\begin{cases} P(\Theta, E) = \sqrt{2E} \cos \Theta \\ Q(\Theta, E) = \sqrt{2E} \sin \Theta \end{cases}. \quad (41)$$

It is clear from this that  $E = H_{\text{osc}}(P, Q)$ . Assuming that this transformation makes sense also after canonical quantization, we would then have:

$$\langle E_m | [H_{\text{osc}}(\hat{P}, \hat{Q}), \Theta(\hat{P}, \hat{Q})] | E_n \rangle = (E_m - E_n) \langle E_m | \Theta(\hat{P}, \hat{Q}) | E_n \rangle, \quad (42)$$

where  $|E_n\rangle$  is a generic eigenstate of the quantum Hamiltonian. This means that the quantized action-angle variables do not satisfy (39). As a consequence, the following result has been shown:

**Theorem 3.** *Canonical quantization depends on the choice of canonical coordinates in terms of which it is performed.*

Note that this result also disproves Claim 1, as it demonstrates that canonical quantization inherently violates general canonical coordinate invariance, a property that was shown in the previous subsection to be the central utility of the Poisson bracket. The operator commutator does not possess this invariance and thus cannot be used to state a quantum version of Theorem 2

### 2.2.2. The failure of the Diracian view of quantization

Here, Claim 2—the idea that quantization is equivalent to ‘turning brackets into commutators’—will be discredited.

**Remark 5.** *The reason for taking the Diracian view seriously from the start is not only due to the CCR. Additionally, the quantum versions of the Hamilton’s equations of motion,*

$$\begin{cases} \frac{i}{\hbar} \left[ H \left( \hat{P}, \hat{Q} \right), \hat{P} \right] = - \frac{\partial H}{\partial Q} \Big|_{(\hat{P}, \hat{Q})} \\ \frac{i}{\hbar} \left[ \hat{T}, \hat{Q} \right] = \frac{\partial H}{\partial P} \Big|_{(\hat{P}, \hat{Q})} \end{cases}, \quad (43)$$

have commutators that play a similar role as the Poisson bracket in Hamiltonian mechanics.

Before disproving Claim 2 we need to further formalize it.

**Definition 4.** *A quantization of a symplectic manifold  $\mathcal{P}$  with associated Poisson algebra  $(C^\infty(\mathcal{P}), \cdot, \cdot)$  is defined as a triple  $\Lambda = (\mathfrak{g}, \mathcal{H}, \Lambda)$ , where  $\mathfrak{g}$  is a unital sub-Lie algebra of  $C^\infty(\mathcal{P})$ ,  $\mathcal{H}$  is a Hilbert space and  $\Lambda : \mathfrak{g} \rightarrow \mathcal{L}(\mathcal{H})$  is a homomorphism, such that:*

- $\Lambda(F)$  is symmetric for all  $F \in \mathfrak{g}$ ,
- The representation  $\Lambda$  is irreducible,
- For all  $F, G \in \mathfrak{g}$  the following equation holds:

$$i\hbar \Lambda(F, G) = [\Lambda(F), \Lambda(G)]. \quad (44)$$

We will for the remainder of this section omit  $\hbar$ , as it serves no other purpose than causing cumbersome notation.

Next, we will demonstrate that canonical quantization does not conform to the definition of a quantization in the sense of Definition 4.

Indeed, the canonical quantization of the simple harmonic oscillator corresponds to a quantization  $\Lambda$  in the sense of Definition 4. In this case, the sub-Lie algebra of the Poisson algebra is spanned by the observables  $P, Q$ , the unit function and  $H_{\text{osc}}$ —as defined by (40)—subject to the relations:

$$\begin{cases} \{P, Q\} = 1 \\ \{H_{\text{osc}}, P\} = -Q \\ \{H_{\text{osc}}, Q\} = P \end{cases}. \quad (45)$$

Because the operator

$$\Lambda(H_{\text{osc}}) - \frac{1}{2} \Lambda(P)^2 - \frac{1}{2} \Lambda(Q)^2 \quad (46)$$

commutes with  $\Lambda(H_{\text{osc}})$ ,  $\Lambda(P)$  and  $\Lambda(Q)$ , and because the representation is irreducible, we can conclude from Schur’s lemma [25] that

$$\Lambda(H_{\text{osc}}) = \frac{1}{2} \Lambda(P)^2 + \frac{1}{2} \Lambda(Q)^2 + c, \quad (47)$$

where  $c \in \mathbb{R}$ , as required for canonical quantization. The same holds true for the free Hamiltonian or the trivial Hamiltonian.

However, as we will demonstrate next, canonical quantization does not generically correspond to a quantization in the sense of Definition 4. To show this, we will consider the particular Hamiltonian

$$H_c = \frac{1}{2}P^2 + \frac{Q^3}{3!}. \quad (48)$$

In this case we have:

$$\begin{cases} \{P, Q\} = 1 \\ \{H_c, P\} = -\frac{Q^2}{2} \\ \{H_c, Q\} = P \end{cases}. \quad (49)$$

In contrast to (40), these relations do not close the algebra  $\mathfrak{g}$ . Hence, one must add  $Q^2$  to  $\mathfrak{g}$ . But it doesn't stop there. Because we then get

$$H_c, Q^2 = 2PQ, \quad (50)$$

meaning that we must also enforce  $PQ \in \mathfrak{g}$ , and so on. It is the occurrence of more such elements that eventually leads to a contradiction, taken in conjunction with the requirement of

$$\Lambda(H_c) = \frac{1}{2}\Lambda(P)^2 + \frac{\Lambda(Q)^3}{3!} + C, \quad (51)$$

for some constant  $C \in \mathbb{R}$ , which is a necessity for  $\Lambda$  to coincide with canonical quantization.

**Theorem 4.** *There does not exist a quantization  $\Lambda$  such that (51) holds.*

**Proof.** We prove this by showing that its existence would lead to a contradiction.

Indeed, if (51) holds, then we calculate that

$$\begin{aligned} \Lambda(Q^2) &= -2i[\Lambda(P), \Lambda(H_c)], \\ &= \Lambda(Q)^2 \end{aligned} \quad (52)$$

and hence that

$$\begin{aligned} \Lambda(PQ) &= -i \left[ \Lambda(H_c), \Lambda\left(\frac{Q^2}{2}\right) \right], \\ &= \Lambda(P)\Lambda(Q) + \frac{i}{2} \end{aligned} \quad (53)$$

In turn, this can be used to calculate

$$\begin{aligned} \Lambda\left(P^2 - \frac{1}{2}Q^3\right) &= -i[\Lambda(H_c), \Lambda(PQ)] \\ &= \Lambda(P)^2 - \frac{1}{2}\Lambda(Q)^3 \end{aligned} \quad (54)$$

and, in turn,

$$\begin{aligned} \Lambda\left(2P^2 + \frac{3}{2}Q^3\right) &= -i \left[ \Lambda\left(P^2 - \frac{1}{2}Q^3\right), \Lambda(PQ) \right] \\ &= \Lambda(P)^2 + \frac{3}{2}\Lambda(Q)^3 \end{aligned} \quad (55)$$

From (54) and (55), we calculate that

$$\begin{aligned}\Lambda(Q^3) &= \frac{2}{5}\Lambda\left(2P^2 + \frac{3}{2}Q^3\right) - \frac{4}{5}\Lambda\left(P^2 - \frac{1}{2}Q^3\right) \\ &= \Lambda(Q)^3.\end{aligned}\quad (56)$$

From (54), we calculate that

$$\begin{aligned}\Lambda(PQ^2) &= -i\frac{2}{5}\left[\Lambda(H_c), \Lambda\left(P^2 - \frac{1}{2}Q^3\right)\right] \\ &= \Lambda(P)\Lambda(Q)^2 - i\Lambda(Q)\end{aligned}\quad (57)$$

From (57), we calculate that

$$\begin{aligned}\Lambda\left(2P^2Q - \frac{1}{2}Q^4\right) &= -i\left[\Lambda(H_c), \Lambda(PQ^2)\right] \\ &= 2\Lambda(P)^2\Lambda(Q) - \frac{1}{2}\Lambda(Q)^4 + 2i\Lambda(P).\end{aligned}\quad (58)$$

From (54) and (57), we calculate that

$$\begin{aligned}\Lambda\left(4P^2Q + \frac{3}{2}Q^4\right) &= -i\left[\Lambda\left(P^2 - \frac{1}{2}Q^3\right), \Lambda(PQ^2)\right] \\ &= 4\Lambda(P)^2\Lambda(Q) + \frac{3}{2}\Lambda(Q)^4 + 4i\Lambda(P)\end{aligned}\quad (59)$$

From these two, we then calculate that

$$\begin{aligned}\Lambda(P^2Q) &= \frac{3}{10}\Lambda\left(2P^2Q - \frac{1}{2}Q^4\right) + \frac{1}{10}\Lambda\left(4P^2Q + \frac{3}{2}Q^4\right) \\ &= \Lambda(P)^2\Lambda(Q) + i\Lambda(P)\end{aligned}\quad (60)$$

From (58), we calculate that

$$\begin{aligned}\Lambda\left(2P^3 - 4PQ^3\right) &= -i\left[\Lambda(H_c), \Lambda\left(2P^2Q - \frac{1}{2}Q^4\right)\right] \\ &= 2\Lambda(P)^3 - 4\Lambda(P)\Lambda(Q)^3 + i6\Lambda(Q)^2.\end{aligned}\quad (61)$$

From (54) and (58), we calculate that

$$\begin{aligned}\Lambda\left(4P^3 + 2PQ^3\right) &= -i\left[\Lambda\left(P^2 - \frac{1}{2}Q^3\right), \Lambda\left(2P^2Q - \frac{1}{2}Q^4\right)\right] \\ &= 4\Lambda(P)^3 + 2\Lambda(P)\Lambda(Q)^3 - i3\Lambda(Q)^2\end{aligned}\quad (62)$$

From these two, we calculate that

$$\begin{aligned}\Lambda(P^3) &= \frac{1}{10}\Lambda\left(2P^3 - 4PQ^3\right) + \frac{2}{10}\Lambda\left(4P^3 + 2PQ^3\right) \\ &= \Lambda(P)^3\end{aligned}\quad (63)$$

Now, we have

$$\begin{aligned}-\frac{i}{9}\left[\Lambda(P^3), \Lambda(Q^3)\right] &= \Lambda(P^2Q^2) \\ &= -\frac{i}{3}\left[\Lambda(P^2Q), \Lambda(PQ^2)\right].\end{aligned}\quad (64)$$

However, we also have—because of (56) and (63)—that

$$-\frac{i}{9} [\Lambda(P^3), \Lambda(Q^3)] = \Lambda(P)^2 \Lambda(Q)^2 - 2i\Lambda(P)\Lambda(Q) - \frac{2}{3}, \quad (65)$$

and—because of (57) and (60)—that

$$-\frac{i}{3} [\Lambda(P^2Q), \Lambda(PQ^2)] = \Lambda(P)^2 \Lambda(Q)^2 - i\frac{2}{3}\Lambda(P)\Lambda(Q) + \frac{1}{3}. \quad (66)$$

(64) together with (65) and (66) imply a contradiction, and hence the proof is completed.  $\square$

From Theorem 4 it directly follows that:

**Corollary 1.** *Canonical quantization does not correspond to a quantization in the sense of Definition 4.*

### 3. A New Perspective on Quantization

In this section, a new perspective on quantization will be presented. Unlike **TQ**, this view does not consider the presence of  $\hbar$  or its manifestation in the CCR as necessary criteria for a quantization. Instead, it is based on the idea that contextuality is the central feature of quantum mechanics and the breaking of general canonical coordinate invariance is at the core of *quantization*. This will be formalized by focusing on flow structures—which consist of a Hamiltonian flow, its associated symmetry group of canonical transformations, and a choice of canonical coordinates—rather than on the general Poisson structure of Hamiltonian mechanics. KvN and OQM will both be revealed to be distinct representations of flow structures. As a result, KvN will have been shown to be equally ‘quantum mechanical’ as OQM in terms of quantization as well as in terms of contextuality.

This section begins with Subsection 3.1, in which the significant achievement of algebraic quantum mechanics—the integration of superselection rules—will be discussed. The application of these superselection rules to the new view of *quantization* presented here will also be explored, and their use in interpreting KvN and OQM as merely distinct representations will be explained. It is assumed that the reader is familiar with algebraic quantum mechanics. Those who are not familiar with the subject are encouraged to consult references [17] for an introduction. In Subsection 3.2, the notion of flow structure is introduced and postulated to correspond to quantization.

#### 3.1. Lessons from algebraic quantum mechanics

In algebraic quantum mechanics, the primary object is the  $C^*$ -algebra  $\mathcal{O}$ . Despite being referred to as the ‘algebra of observables’, the elements of  $\mathcal{O}$  may not directly correspond to physical observables. For instance, in the case of the  $C^*$ -algebraic formulation of the CCR-algebra,  $\mathcal{O}$  is not generated by  $\hat{p}$  and  $\hat{q}$  subject to the restriction

$$\hat{p}\hat{q} - \hat{q}\hat{p} = i\hbar. \quad (67)$$

Instead,  $\mathcal{O}$  is generated by its ‘integrated version’—the Weyl group—formally created by the elements  $X(t) := e^{it\hat{p}}$  and  $Y(t) := e^{it\hat{q}}$ . This is because the elements of a  $C^*$ -algebra must be bounded, while  $\hat{p}$  and  $\hat{q}$  are not. This article does not fully commit to the algebraic view of quantum mechanics as the relevant observables must be mapped to fit the description of a  $C^*$ -algebra. While it is true that both OQM—via the ‘integrated CCR’—as well as KvN [35] can be formulated in terms of algebraic quantum mechanics, they end up corresponding to different algebraic structures. The hypothesis of this article is that they fundamentally corresponds to the same structure, only being separated at the level of representations of this structure.

The view that quantization corresponds to a mapping of a Hamiltonian mechanical (sub)structure to a  $C^*$ -algebraic one is hence not pursued. This does not imply that the algebraic formulation is completely disregarded, as it is mathematically inherent to the quantum formalism. What is challenged is the notion that the  $C^*$ -algebraic structure holds a privileged position in terms of fundamental

principles. Instead, group structures are here postulated to rather hold such a more privileged position. In line with this, in the next subsection, the group theoretical aspects of Hamiltonian mechanics with regards to *quantization* will be emphasized. In doing so, what is arguably the greatest achievement of the algebraic approach [17]—the incorporation of superselection rules [10]—will be incorporated to interpret the difference between OQM and KvN as merely inequivalent representations of the same structure.

In the algebraic approach, one considers unitary representations of  $\mathcal{O}$ , which leads to the traditional Hilbert space formulation. If the unitary representation is reducible, it is said to be subject to superselection rules and its irreducible subrepresentations are referred to as superselection sectors. On the other hand, in the traditional Hilbert space formalism, two subspaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$  of  $\mathcal{H}$  are considered superselection sectors if they are separated by a superselection rule. This means that for all states  $\psi_A \in \mathcal{H}_A$  and  $\psi_B \in \mathcal{H}_B$ ,

$$\langle \psi_A, O \psi_B \rangle = 0, \quad (68)$$

holds for all observables  $O$ . As a result, there is no observable difference between the pure state

$$c_A \psi_A + c_B \psi_B, \quad (69)$$

and the corresponding mixed state

$$|c_A|^2 |\psi_A\rangle \langle \psi_A| + |c_B|^2 |\psi_B\rangle \langle \psi_B|. \quad (70)$$

As there certainly exist self-adjoint operators  $A$  for which instead

$$\langle \psi_A, A \psi_B \rangle \neq 0, \quad (71)$$

for instance

$$A = |\psi_A\rangle \langle \psi_B| + |\psi_B\rangle \langle \psi_A|, \quad (72)$$

it is clear that the meaning of superselection is that not every self-adjoint operator corresponds to an actual observable.

We can reconcile the algebraic and Hilbert space perspectives on superselection by noting that if  $\mathcal{H}_A$  and  $\mathcal{H}_B$  are irreducible subrepresentations of  $\mathcal{O}$  that together form an orthogonal decomposition of  $\mathcal{H}$ , then equation (68) holds for all  $O \in \mathcal{O}$ .

The occurrence of superselection rules is explained in the algebraic approach as follows: If the commutant

$$\rho(\mathcal{O})' := \{A \in \mathcal{B}(\mathcal{H}) : [A, \rho(O)] = 0, \forall O \in \mathcal{O}\}, \quad (73)$$

of a representation  $\rho$  of  $\mathcal{O}$  is non-trivial—meaning it contains elements other than proportional to the identity—then  $\rho$  is subjected to superselection rules, as stated in [10,36]. This is due to Shur's lemma, which says that  $\rho$  is irreducible if and only if its commutant is trivial. In the next subsection, we will implement this concept of superselection.

In addition, we do not limit our observables to those in  $\mathcal{O}$  alone. We also allow observables that correspond to elements of the commutant  $\rho(\mathcal{O})'$ —which are referred to as **superselection observables**—to be included. These observables can be related to specific values in superselection sectors. For instance, the charge of a particle is a archetypical example of a superselection observable, as it is considered unphysical to be in a superposition of different charges because of the conservation of charge.

**Remark 6.** *Based on the traditional purely Hilbert space account of superselection rules, it is clear that there is an intimate relationship between superselection rules and contextuality. For example, regarding the contextuality claimed by the author to occur in KvN in a previous work [11], it is possible that this effect could be eliminated if one posited that the eigenspaces of the Liouvillian are superselection sectors. However, it is unclear what*

justification such a superselection rule could have. Moreover, this would necessarily result in the considered Hilbert space being different from that of KvN, thus one would no longer be doing KvN.

### 3.2. The flow structure and its representations

In this subsection, we postulate that *quantization* corresponds to a substructure of Hamiltonian mechanics associated with a chosen Hamiltonian flow, referred to as a 'flow structure'. In the introduction of this article, KvN was presented as a unitary representation of the Hamiltonian flow, which is true for OQM as well. However, a unitary representation of a flow alone simply represents  $\mathbb{R}$ , therefore, some additional structure is required. Hinted in Remark 5, OQM satisfies the quantum version of Hamilton's equations of motion, which requires at least a pair of self-adjoint operators corresponding to the quantum analogues of  $P$  and  $Q$ . Moreover, there is an inherent symmetry of canonical transformations associated with each Hamiltonian flow. This structure is postulated to correspond to a quantization of Hamiltonian mechanics.

We will demonstrate that KvN and OQM correspond to unitary representations of flow structures. Similar to algebraic quantum mechanics, superselection rules are implemented, leading to the conclusion that KvN and OQM correspond to different superselection sectors.

We will start by defining *inherent symmetry of a Hamiltonian flow*.

**Definition 5.** *The inherent symmetry of a Hamiltonian mechanical system  $(\mathcal{P}, U)$ , where  $\mathcal{P}$  is a Hamiltonian phase space and  $U$  is a Hamiltonian flow is the group*

$$\mathcal{G}_U := \{G \in \text{Symp}(\mathcal{P}) : \text{for all } t \in \mathbb{R}, U_t \circ G = G \circ U_t\}. \quad (74)$$

**Remark 7.** *Note that  $U$  is a subgroup of  $\mathcal{G}_U$ , and that it moreover by definition is in the center of it.*

Next we define *flow structure*.

**Definition 6.** *Let  $\mathcal{P}$  be a Hamiltonian phase space. A **flow structure** on  $\mathcal{P}$  is a pair*

$$(U, (P, Q)), \quad (75)$$

*where  $U$  is a Hamiltonian flow and  $(P, Q)$  is a choice of canonical coordinates.*

**Remark 8.** *Note that inherently associated to the flow structure  $(U, (P, Q))$  there is also the group  $\mathcal{G}_U$  of inherent symmetries of  $U$ .*

The flow structures of a Hamiltonian phase space  $\mathcal{P}$  are deemed to be the essential sub-structure of  $\mathcal{P}$  that is relevant to quantization. In other words, these flow structures are the structures of  $\mathcal{P}$  that must be represented in the formalism of quantum mechanics. It is important to note that, in contrast to the traditional view, quantization is not inherently about mapping the full Hamiltonian structure of classical mechanics into the formalism of quantum mechanics. Instead, a part of quantization involves singling out the particular type of flow structure.

Next, we define how flow structures are represented in the formalism of quantum mechanics.

**Definition 7.** *A **flow representation** of a flow structure  $(U, (P, Q))$  is a double  $(\Lambda, \lambda)$ , where  $\Lambda$  is a unitary representation of  $\mathcal{G}_U$  on a Hilbert space  $\mathcal{H}$ ,  $\lambda$  is a mapping,*

$$\lambda : F \in \{P \circ G : G \in \mathcal{G}_U\} \cup \{Q \circ G : G \in \mathcal{G}_U\} \mapsto \lambda(F), \quad (76)$$

*where each  $\lambda(F)$  is self-adjoint on  $\mathcal{H}$  such that:*

- $\lambda(F \circ G) = \Lambda(G)^* \lambda(F) \Lambda(G)$  (77)
- $$\begin{cases} \frac{d}{dt} \Big|_{t=0} \lambda(P \circ G \circ U_t) = - \frac{\partial \mathbb{H}}{\partial q} \Big|_{(\lambda(P \circ G), \lambda(Q \circ G))}, \\ \frac{d}{dt} \Big|_{t=0} \lambda(Q \circ G \circ U_t) = \frac{\partial \mathbb{H}}{\partial p} \Big|_{(\lambda(P \circ G), \lambda(Q \circ G))} \end{cases},$$
 (78)

where  $\mathbb{H}$  is the function such that  $H = \mathbb{H} \circ (P, Q)$ .

**Remark 9.** Note, because  $U$  is in the center of  $\mathcal{G}_U$ —Remark 7—any flow representation must be such that

$$\begin{cases} \Lambda(G)^* \frac{\partial \mathbb{H}}{\partial q} \Big|_{(\lambda(P), \lambda(Q))} \Lambda(G) = \frac{\partial \mathbb{H}}{\partial q} \Big|_{(\lambda(P \circ G), \lambda(Q \circ G))}, \\ \Lambda(G)^* \frac{\partial \mathbb{H}}{\partial p} \Big|_{(\lambda(P), \lambda(Q))} \Lambda(G) = \frac{\partial \mathbb{H}}{\partial p} \Big|_{(\lambda(P \circ G), \lambda(Q \circ G))} \end{cases},$$
 (79)

which is a non-trivial relation in the case of  $\frac{\partial \mathbb{H}}{\partial p}$  and  $\frac{\partial \mathbb{H}}{\partial q}$  not being of polynomial form.

Now we can fully state the suggested reformulation of quantization:

**Postulate 1.** A **quantization** of a Hamiltonian phase space  $\mathcal{P}$  corresponds to a flow representation  $(\Lambda, \lambda)$  of a flow structure  $(U, (P, Q))$  on  $\mathcal{P}$ .

Before demonstrating that both KvN and OQM correspond to flow representations—i.e., to quantizations in the sense of Postulate 1—we will define what it means for a flow representation to be irreducible. We will do this in terms of equivalences of flow representations. Therefore, we need to first define what is meant by *equivalence*.

**Definition 8.** Let  $(\Lambda, \lambda)$  and  $(\Lambda', \lambda')$  be two flow representations of  $(U, (P, Q))$ . A **flow representation isomorphism** (FRI) from  $(\Lambda, \lambda)$  to  $(\Lambda', \lambda')$  is a unitary map

$$\mathcal{V} : \mathcal{H} \rightarrow \mathcal{H}'$$
 (80)

such that

$$\Lambda'(G) = \mathcal{V} \Lambda(G) \mathcal{V}^*,$$
 (81)

for all  $G \in \mathcal{G}_U$ , and

$$\begin{cases} \lambda'(P) = \mathcal{V} \Lambda(P) \mathcal{V}^* \\ \lambda'(Q) = \mathcal{V} \Lambda(Q) \mathcal{V}^* \end{cases}.$$
 (82)

$(\Lambda, \lambda)$  and  $(\Lambda', \lambda')$  are **equivalent** if there exists an IFR from one to the other. An FRI from  $(\Lambda, \lambda)$  onto itself is called a **flow representation automorphism** (FRA).

In representation theory, Schur's lemma states that any intertwining operator between two irreducible representations on the same space must be proportional to the identity. Using this analogous statement, we will define *irreducibility* in the context of flow representations.

**Definition 9.** A flow representation  $(\Lambda, \lambda)$  is **irreducible** if all its FRAs are proportional to the identity, otherwise it is **reducible**.

In analogy with algebraic quantum mechanics we define the following:

**Definition 10.** A flow representation  $(\Lambda, \lambda)$  of  $(U, (P, Q))$  on  $\mathcal{H}$  is subjected to **superselection rules** if there exists a self-adjoint operator  $A$  on  $\mathcal{H}$  such that  $A \not\propto \text{id}_{\mathcal{H}}$  and

$$[\Lambda(\mathcal{G}_U), A] = [\lambda(P), A] = [\lambda(Q), A] = 0. \quad (83)$$

Next we show that the occurrence of a superselection rule is equivalent to the flow representation being reducible.

**Theorem 5.** A flow representation  $(\Lambda, \lambda)$  is subjected to superselection rules if and only if it is reducible.

**Proof.** First, if  $(\Lambda, \lambda)$  is subjected to superselection rules, then there exists non-trivial self-adjoint operator  $A$  such that (83) holds.  $e^{iA}$  then defines an non-trivial FRA on  $(\Lambda, \lambda)$ , and hence it must be reducible.

Second, if  $(\Lambda, \lambda)$  is reducible, then there exists a non-trivial FRA  $\mathcal{V}$ . To  $\mathcal{V}$  we can associate a non-trivial self-adjoint operator  $A$  such that  $e^{iA}$ , which consequently must satisfy (83). Hence making  $(\Lambda, \lambda)$  subjected to a superselection rule.  $\square$

Note that the set of FRAs associated with a flow representation  $(\Lambda, \lambda)$  has the structure of a group. We denote this group by  $\mathcal{R}_{\Lambda, \lambda}$ , referring to it as its **degeneracy group**. A flow representation is then irreducible if and only if

$$\mathcal{R}_{\Lambda, \lambda} = \{e^{i\theta} \text{id}_{\mathcal{H}} : \theta \in [0, 2\pi)\}. \quad (84)$$

*Irreducibility*, in a way, is hence similar to there being no redundancies. Following this analogy, we can hypothesize how a superselection rule can be removed even if the flow representation is reducible.

**Hypothesis 1.** A superselection rule of a flow representation  $(\Lambda, \lambda)$  can be removed by connecting its degeneracy group  $\mathcal{R}_{\Lambda, \lambda}$  with an actual symmetry, that is, by finding a physically meaningful group  $\mathcal{G}$  and a unitary representation  $\rho$  such that

$$\rho(\mathcal{G}) = \mathcal{R}_{\Lambda, \lambda}. \quad (85)$$

Although we will make a reference to this hypothesis in the context of KvN later, we will not delve into its full meaning. Nonetheless, it is worth mentioning to avoid giving the impression that flow structures are the final word in some sense.

Next we move on towards showing that both KvN and OQM correspond to flow representations.

**Example 1.** In KvN is a flow representation  $(\Lambda, \lambda)$  of  $(\mathcal{G}_U, (P, Q))$  for which

$$\mathcal{H} = L^2(\mathcal{P}, d\mu), \quad (86)$$

with  $\mu$ , any  $\mathcal{G}_U$ -invariant measure on  $\mathcal{P}$ —such as  $dPdQ$  or  $dPdQ\rho \circ H$ , for instance—and

$$\Lambda(G)\psi := \psi \circ G^{-1} \quad (87)$$

for all  $G \in \mathcal{G}_U$  and  $\psi \in \mathcal{H}$ , where, for any  $F \in C^\infty(\mathcal{P})$ , we define

$$\lambda(F)\psi := F\psi. \quad (88)$$

It can be easily verified that

$$\Lambda(G)^* \lambda(F) \Lambda(G)\psi = \lambda(F \circ G)\psi, \quad (89)$$

for all  $G \in \mathcal{G}_U$  and thus by replacing  $F$  with any  $P \circ G'$  and  $Q \circ G'$ ,  $G' \in \mathcal{G}_U$ , respectively, and  $G$  with any  $U_t$ , it is shown that (78) is satisfied. KvN is a flow representation of  $(\mathcal{G}_{(\mathcal{P}, U)}, (P, Q))$ .

**Remark 10.** Note that KvN, with the choice of  $dPdQ$  as the integration measure, defines a flow representation of any flow structure on  $\mathcal{P}$ . However, if the integration measure is chosen as  $dPdQ\rho \circ H$ , this is no longer the case because the measure is not invariant under all inherent symmetries  $\mathcal{G}_{U'}$  of any Hamiltonian flow  $U'$ . Nonetheless, it could still potentially be a flow representation of  $(U, (P', Q'))$  for any choice of canonical coordinates  $(P', Q')$ .

Referring to the choice of  $dPdQ$  as integration measure as the **full KvN**, we can see that this flow representation is subjected to superselection rules. This is because the full KvN is a reducible flow representation. For every function  $h : \mathbb{R} \rightarrow \mathbb{R}$ ,

$$\mathcal{V}_h \psi := e^{ih \circ H} \psi, \quad (90)$$

defines an FRA on the full KvN.

However, by considering the measure  $(\delta_E \circ H)dPdQ$ , where, for any  $E \geq 0$ ,

$$\delta_E(\omega) = \delta(H(\omega) - E), \quad (91)$$

we observe that the FRAs  $\mathcal{V}_h$  take the form of  $e^{ih(E)}I$ . A closer look reveals that this symmetry corresponds to the large degeneracy present in the full KvN with regards to the eigenstates of its generator of time evolution—the Liouvillian  $\mathcal{L}$ .

The Liouvillian satisfies:

$$\mathcal{L}\psi = i\{H, \psi\}. \quad (92)$$

Working formally, ignoring the possibility of other constants of motion besides  $H$ , a generic eigenstate  $\phi$  with eigenvalue  $L$  can be expressed as:

$$\phi = e^{-iL\Omega} f \circ H, \quad (93)$$

where  $\Omega$  satisfies:

$$\{H, \Omega\} = 1. \quad (94)$$

There is a huge degeneracy in the choice of  $f$ , with the only restriction being that the state must have finite norm. This degeneracy is represented by the symmetry (90). Based on Hypothesis 1, one may speculate about the physical meaning of this symmetry, otherwise the full KvN is subjected to a superselection rule with  $H$ —typically corresponding to the energy observable—as the superselection observable.

In contrast, KvN with the integration measure of  $dPdQ\rho_E \circ H$  is irreducible and not subjected to a superselection rule. This corresponds to fixing the value of the superselection observable  $H$  at  $E$ . This measure corresponds to the microcanonical ensemble in classical statistical mechanics. The appearance of this superselection rule might seem natural in that context, as it is equivalent to the common assumption [37] that an isolated system—such as the system + heat reservoir—always behaves according to the microcanonical ensemble.

**Remark 11.** Note that the microcanonical ensemble here is a result of a superselection rule, not from some principle of ‘equal prior probability’.

**Remark 12.** The KvN formalism has been interpreted in the context of statistical mechanics, but this interpretation is not inherent to KvN. Statistical mechanics relies on the assumption of a large number of particles, while KvN does not make this assumption.

Next we show that OQM is a flow representation.

**Example 2.** We consider a traditional Hamiltonian function  $H$  and coordinates  $(P, Q)$  with respect to which the Hamiltonian is of traditional spherically symmetric form,

$$H(p, q) = \frac{1}{2m}|p|^2 + V(|q|). \quad (95)$$

That is,  $\mathcal{G}_U$  is generated by the flow  $U$  and the canonical transformations of the form

$$(P, Q) \mapsto (R^\perp P, RQ), \quad (96)$$

where  $R$  belongs to the group  $SO(3)$  of rotation matrices. We consider the Hilbert space  $L^2(\mathbb{R}^3)$ . Where we define

$$\begin{cases} (\lambda(P_n)\psi)(x) := ci\partial_n\psi(x) \\ (\lambda(Q_n)\psi)(x) := x_n\psi(x) \end{cases} \quad (97)$$

Because  $U$  and every rotation (96) commute, we may simply define  $\Lambda$  as

$$\begin{cases} \Lambda(U_t) := e^{-it\frac{1}{\hbar}H(\lambda(P), \lambda(Q))} \\ \Lambda(R)\psi := \psi \circ R^\perp \end{cases} \quad (98)$$

We may then simply define

$$\begin{cases} \lambda(P_n \circ G) := \Lambda(G)^*\lambda(P_n)\Lambda(G) \\ \lambda(Q_n \circ G) := \Lambda(G)^*\lambda(Q_n)\Lambda(G) \end{cases} \quad (99)$$

for all  $G \in \mathcal{G}_U$ . It is a straightforward calculation to show (78), which may be found in any textbook on quantum mechanics, say, [34]. So indeed, OQM corresponds to a flow representation.

Note that the rotation symmetry in Example 2 is familiar from the quantization of the coulomb potential, where the degeneracy of energy levels is described by the unitary representation of the rotation group [34]. It is well known that, in the absence of spin, the rotation group describes the full degeneracy of the quantum Hamiltonian. Furthermore, in OQM as any operator that commutes with both  $\lambda(P)$  and  $\lambda(Q)$  must be proportional to the identity [34], OQM is irreducible as flow representation, and hence not subjected to a superselection rule.

**Remark 13.** The reason for choosing a traditional Hamiltonian in Example 2 is to avoid the issue with the ordering ambiguity caused by the CCR. This issue has not been resolved by this view of quantization, but that was neither its intended purpose.

Note: If two flow representations  $(\Lambda, \lambda)$  and  $(\Lambda', \lambda')$  are equivalent, then any FRI  $\mathcal{V}$  between them must be such that

$$[\lambda'(P), \lambda'(Q)] = \mathcal{U}[\lambda(P), \lambda(Q)]\mathcal{U}^*. \quad (100)$$

We use this to prove the following result:

**Theorem 6.** KvN and OQM are mutually inequivalent flow representations.

**Proof.** Assume that  $(\Lambda, \lambda)$  is of KvN-type—i.e that  $\lambda(P)$  and  $\lambda(Q)$  commute—and that  $(\Lambda, \lambda)$  is of OQM-type—i.e that  $\lambda(P)$  and  $\lambda(Q)$  satisfy the CCR. If they are equivalent, there must be a an FRI such that (100) holds, which is a contradiction.  $\square$

As stated in Theorem 6, KvN and OQM represent different superselection sectors. This provides the possibility of interpreting  $i[\lambda(P), \lambda(Q)]$  as a superselection observable, as it commutes with the flow structure in both KvN and OQM. This viewpoint could offer a way to include  $\hbar$ -dependence in the flow structure, similar to Deformation quantization [25] or Plain mechanics [38]. However,

these approaches appear to still rely on the belief that  $\hbar$  is the essence of quantum mechanics and that proper quantum phenomena cannot occur without it. This belief is challenged in the author's previous work [11]. The quantization approach presented here incorporates these findings, while Deformation quantization and Plain mechanics seem unable to do so.

#### 4. Conclusion

This article has challenged the traditional view of quantization, proposing a new and novel perspective instead. The traditional view, based on a Diracian interpretation, relies on similarities between the Poisson bracket and the commutator, such as the correspondences:

$$\{P, Q\} = 1 \longleftrightarrow \frac{1}{i\hbar} [\hat{P}, \hat{Q}] = I \quad (101)$$

and

$$\begin{cases} \{H, P\} = -\partial_Q H \\ \{H, Q\} = \partial_P H \end{cases} \longleftrightarrow \begin{cases} \frac{1}{i\hbar} [\hat{H}, \hat{P}] = -\partial_Q H|_{(\hat{P}, \hat{Q})} \\ \frac{1}{i\hbar} [\hat{H}, \hat{Q}] = \partial_P H|_{(\hat{P}, \hat{Q})} \end{cases} . \quad (102)$$

However, this view is not inherent to the modern, probabilistic interpretation of quantum mechanics—in which contextuality is the essential phenomenon—as the correspondence (101) is merely a particular manifestation of contextuality, not the phenomenon itself.

Through a Groenewold-van Hove-type theorem, it was demonstrated that any formalization of the Diracian view as a unitary irreducible representation of a sub-Lie algebra of the Poisson algebra is plagued by the well-known ordering ambiguity and therefore cannot exist. Additionally, it was shown that OQM violates the canonical coordinate invariance central to the utility of the Poisson bracket in Hamiltonian mechanics. Rather than interpreting this and Groenewold-van Hove-type theorems as posing problems to the Diracian view to be worked around, a new view of *quantization* was suggested in which the breaking of general canonical coordinate invariance is instead embraced, (101) is discarded and (102) is interpreted as indicative of a unitary representation of the Hamiltonian flow.

In this new perspective, quantization corresponds to the selection of a flow structure that consists of a Hamiltonian flow, its associated symmetry group of canonical transformations, and a choice of canonical coordinates. KvN and OQM have been shown to correspond to different flow representations. This view of quantization is consistent with the author's prior work, in which KvN was demonstrated to exhibit contextuality and should therefore be considered a proper quantum mechanical theory. Additionally, it implements the principle of superselection, where KvN and OQM correspond to different superselection sectors and  $i[\lambda(P), \lambda(Q)]$  may serve as the superselection observable. Furthermore, it was noted that the superselection sectors of both KvN and OQM break general canonical coordinate invariance, fulfilling the general objective of quantization as being inherently connected with the breaking of this invariance.

In addition to aligning with the modern, probabilistic interpretation of quantum mechanics, this new approach to quantization differs from the traditional one in that it proposes that the classical-to-quantum transition may have a physical significance, whereas in the traditional view, it is merely seen as an algorithmic procedure. This new perspective suggests that quantization is inherently linked to the breaking of canonical coordinate invariance and that the possibility of  $i[\lambda(P), \lambda(Q)]$  serving as a superselection observable gives direct physical meaning to the classical-to-quantum transition. For instance, the breaking of canonical coordinate invariance may reflect the manifestation of the 'particle picture'. Although Hamiltonian mechanics may describe a system using any canonical coordinates, it is seems that describing the system in terms of the spatial positions and momenta of its constituents is 'more real'. Perhaps quantization functions to make this 'realness' manifest.

In contrast, the traditional view is based on a reductionist perspective, where the physical significance lies in the quantum-to-classical direction, in the sense of the classical limit. It is

thus suggested that this new perspective on quantization is best understood within the context of non-reductionist views on physics and science [1,3,27–30,39,40].

**Funding:** This research received no external funding.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable

**Acknowledgments:** I would like to thank Andrei Khrennikov for stimulating discussions and comments. I would also like to thank my wife, this article would not have been possible with out her support when writing got tough.

**Conflicts of Interest:** The author declare no conflict of interest.

## Abbreviations

The following abbreviations are used in this manuscript:

TQ	Traditional view of <i>quantization</i>
CCR	Canonical commutation relations
KvN	Koopman-von Neumann formulation
OQM	Ordinary non-relativistic quantum mechanics
FRI	Flow representation isomorphism
FRA	Flow representation automorphism

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