POTENTIAL CANONICAL FRAMEWORK FOR QUANTUM-CLASSICAL DYNAMICS

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Dedication

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Abstract

Dynamical brackets lie at the heart of fundamental physical theories. They are Lie brackets that obey the Leibniz rule with respect to a suitable composition product. The pair "composition product" and "dynamical bracket" define a formal dynamical structure that is common to classical and quantum mechanics. Without properties like the Jacobi identity and the Leibniz rule, the consistency of a dynamical framework cannot be guaranteed.

This work investigates the possibility of combining quantum and classical dynamics into a single, consistent framework. We generalize previous attempts and discuss no-go theorems that assert their inconsistency. We show that the Jacobi identity and Leibniz rule are satisfied provided there exists an associative product for hybrid variables. This condition motivates the construction of associative subalgebras over which quantum-classical dynamics is consistent: perhaps hybrid observables are constrained to belong to such algebras. If so, only certain interactions between quantum and classical systems would be allowed.

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Chapter 1

Introduction

Quantum mechanics is the fundamental framework for the description of almost all matter and interaction, with gravity as a notable exception. Replacing classical theories, quantum mechanical theories have been successfully constructed and experimentally verified for all known fundamental particles and the forces acting on them. Classical mechanics, the successful framework for relatively larger objects, is believed to be contained in quantum mechanics as a limiting case.

Conceptually, it follows that quantum mechanics is sufficient to describe all natural phenomena apart from gravity. Practically, physicists resort to some form of a mixed description in many cases. It is well known that an exact quantum mechanical calculation of the spectrum of atoms more complicated than hydrogen is a difficult task. Even in the simple case of the hydrogen atom, the electromagnetic field mediating the interaction between the nucleus and the electron is treated in a simplified manner which is ultimately classical.

Standard textbook examples of simple quantum mechanical systems are examples of *mixed* quantum-classical systems: a quantum particle in an external potential [1]. From a fundamental point of view, an external potential must have a source that obeys a dynamical law. In textbook quantum mechanics, the external field has a definite spatial arrangement and time-variation (velocity) of such arrangement; it is classical. This description, baked into elementary quantum mechanics, is sufficient for the description of a wide variety of phenomena, avoiding the complications of a

full quantum description.

The use of a simplified quantum-classical description is inevitable when one deals with a collection of atoms. Many-body problems are notoriously difficult to solve and simplifying arguments are needed for useful predictions. Indeed, many models for such systems rely, among other assumptions, on the treatment of atomic nuclei as classical objects [2, 3].

The mixing of quantum and classical mechanics is also useful for purposes other than computational simplicity. General relativity is a classical theory that has resisted quantization from the beginning and remains stubbornly difficult to this day. Nevertheless, various approaches to quantum gravity benefit from the study of quantum field theory on curved backgrounds, a mixed quantum-classical analysis. The study of the interface between quantum and classical systems is thus beneficial for conceptual as well as practical endeavours.

In the familiar previous examples, only the classical part of the system (be it an external potential, a heavy nucleus or a spacetime background) acts on the quantum part, but not the other way around. It can be argued that the scale of the classical system is "large enough" that it is not affected by the small quantum systems it coexists with. This is a valid approximation for many interesting cases, but not all of them. An approximation that captures mutual interaction between the two subsystems, instead of the one-sided action of the "large" on the "small", can offer interesting results.

For example, in the BCS theory, an attractive interaction between electrons is used for the description of superconductivity. The effective attractive potential arises from an electron-phonon interaction in crystals [4]. That is, an *inter*-action between the tiny electron and the massive nuclei. The realization of the possibility that the small acts back on the large allowed for the understanding of nontrivial phenomena with far-reaching potential applications.

What if the "large" is approximated as "classical"? If that approximation provides a computationally less demanding model, while allowing for the mutual interaction between classical and quantum degrees of freedom, then interesting results are expected. Approximations of this type (mixing classical and quantum degrees of freedom) are useful in chemical physics for example (see [3] for a review).

A more striking example of quantum systems acting on classical ones is the orthodox/Copenhagen view of the measurement process. In Bohr's view of quantum mechanics, a measuring device *must* be modeled as classical, even though classical mechanics *is* a limiting case of quantum mechanics [5]. For the measuring device to record any measurement, it must have been acted upon by the quantum system it measures. A dynamical framework capable of describing such action could, at least in principle, provide a mechanism for the process of quantum measurement.

The inclusion of quantum *back-reaction* on the classical subsystem would have important implications for cosmology as well. Density perturbations in the early universe are modeled to have seeded the structure formation of galaxies and galaxy clusters. The origin of these perturbations, however, is not well-understood. In inflationary models of the universe, an inflaton field drives an early exponential expansion of the universe. While treating spacetime classically, the quantum nature of the inflaton field is invoked to generate density perturbations through quantum fluctuations in the inflaton field [6, 7, 8, 9, 10]. These quantum fluctuations of the matter field would, in turn, cause spacetime perturbation, and *that* we cannot model. These perturbations are put in by hand in an ad hoc manner that is inconsistent with general relativity and quantum mechanics [11].

In the absence of a universally agreed-upon theory of quantum gravity, a consistent framework for quantum-classical interaction may offer insight for early universe cosmology. In fact, a consistent description of phenomena where both gravity and the quantum nature of matter are relevant could be useful for the study of singular-

ities. Can we consistently model perturbations after the big bang? What happened before the big bang (if that is a meaningful question)? What happens to cups of tea falling into black holes? *If* consistent quantum-classical dynamics exists, it can provide an illuminating first approximation to full quantum gravity. *If* consistent quantum-classical dynamics exists, it might even allow for the logical possibility of treating gravity as fundamentally classical.

Attempts at a quantum-classical framework have been proposed since the 1980's with the work of Aleksandrov [12], Gerasimenko [13], and Boucher and Traschen [11]. These attempts inspire the work presented here. They describe quantum-classical dynamics in terms of a *hybrid bracket* which is desired to mimic the role of quantum commutators and classical Poisson brackets. These proposals, among others, have been criticized by Salcedo and Sahoo and collaborators in [14, 15, 16, 17, 18] on the basis of inconsistency.

To see what is meant by dynamical consistency, we look at the formal structure common to both quantum and classical dynamics. That formal dynamical structure is based on a *dynamical bracket* that is a Lie bracket that obeys the Leibniz rule with respect to some *composition product*. A composition product is an associative, generally noncommutative binary operation that composes two dynamical variables into a third one. Operator quantum mechanics has operators on Hilbert space as its dynamical variables, noncommutative operator product as its composition product, and essentially the commutator as its dynamical bracket. Classical mechanics has functions on phase space as its dynamical variables, familiar commutative pointwise multiplication as its composition product, and the Poisson bracket as its dynamical bracket. The uncertainty (or lack thereof) is tied to the commutativity of the composition product.

This formal structure is desired since many tools of theoretical physics have been developed around it. It is robust enough that it is applicable to vastly different

theories, from nonrelativistic classical mechanics to general relativity to quantum physics. The necessity of this formal structure for the consistency of a dynamical framework is discussed in Ch. 2. We expect a consistent hybrid quantum-classical framework to possess the same formal structure.

The no-go theorems in [14, 15, 16, 17, 18] found that the hybrid dynamical bracket proposed in [11] (among others) lacks the crucial properties of obeying the Jacobi identity and the Leibniz rule, implying its inconsistency. These negative results leave no option for quantum-classical mechanics but to be an approximation of limited validity. For example, they have been used to argue against the possible combination of quantum mechanics and classical gravity in a meaningful way (see [19] and references therein).

The main goal of this work is to explore possible paths towards the resolution of this problem. Analyzing the aforementioned no-go theorems, we found that the origin of violation of the Jacobi and Leibniz properties can be traced to one mathematical condition. Defining the hybrid bracket in terms of the commutator of a certain product, we show that *if* that product is associative, the Jacobi identity is identically satisfied. The bracket will also, as an identity, obey the Leibniz rule with respect to said product, suggesting its role as a composition product for hybrid variables. These results are presented in the preprint [20].

This realization of the single condition for "consistency" of the dynamical bracket provides a fresh angle for inspecting the problem. If the associativity of the hybrid composition product can be secured, then a hybrid bracket can, in principle, define consistent hybrid dynamics.

In deriving and discussing the consistency condition, we chose the phase space formulation of quantum mechanics to approach the problem. Phase space quantum mechanics uses the same entities as that of classical mechanics, unifying the language and providing a straightforward study of the quantum-classical bracket. Further, it

provides a relatively simple procedure for constructing possible candidates for the hybrid composition product. The results can be translated to familiar operator language.

We find that simple schemes for constructing the hybrid product yield a generally nonassociative one. At first glance, this seems to merely restate the aforementioned no-go theorems in more general terms. However, as mentioned earlier, the realization of the precise mathematical condition for consistency may hint at a possible circumvention of these no-go theorems. From the associativity condition branch off two paths worth exploring. One path is the construction of a nontrivial, generally associative composition product. While it is not proven that this task is impossible, it is, like its desired outcome, nontrivial.

The other path is to impose a restriction on the allowed hybrid dynamical variables, that they form an associative subalgebra along with a given composition product. Venturing down this road reveals some interesting possibilities. For example, a restriction on hybrid dynamical variables implies a restriction on admissible quantum-classical interactions. Further, depending on the setup, it may also impose phase space constraints which could point us towards gauge theories [21, 22].

While the associativity condition for the hybrid composition product helps us rethink the construction of quantum-classical dynamics, more work remains to be done. For example, the hybrid composition product, along with the restrictions it imposes, requires physical interpretation. What would hybrid variables mean, other than interaction terms in the Hamiltonian? What are the allowable transformations and symmetries of hybrid mechanics? On the other hand, how can we define an appropriate quantum-classical hybrid "state"? Concrete examples need to be calculated and compared to fully quantum and fully classical treatments. We may have found a sign, but we are a long way from a complete map.

This thesis is divided into three parts. In Ch. 2 we introduce Hamiltonian classical

mechanics with an emphasis on its formal structure. The general properties of a dynamical bracket are discussed along with their necessity for a consistent description.

Ch. 3 carries the same phase space formal structure of the preceding chapter to quantum mechanics. We summarize the generalizations needed to allow for a suitable description of quantum phenomena. The relation to operator quantum mechanics is outlined in order to make connection with familiar concepts. An important step towards hybrid dynamics is a clear and controlled application of the classical limit of quantum mechanics. We discuss this limit in the operator and phase space formulations highlighting the advantage of the latter. Since it provides a conceptual motivation for studying quantum-classical interaction, we briefly present the process of quantum measurement and the orthodox/Copenhagen account of it.

In Ch. 4 we introduce hybrid quantum-classical mechanics and the main results of this work. After motivating the need for the hybrid framework, we detail the derivation of the quantum-classical bracket through the application of a partial classical limit. An alternative formal construction of the bracket, bypassing the classical limit step is also discussed. We find a generalized bracket that contains the bracket proposed in [11] as a special case. We then discuss general properties of the bracket as derived, without extra conditions imposed, and show possible useful applications for it. Following that, we discuss the consistency of the bracket and the no-go theorems of [15, 16, 18], before introducing the mathematical condition for the bracket's consistency: the associativity of the hybrid composition product. We then move on to show a proof of concept for the use of such a new realization in the search for a consistent quantum-classical dynamical framework. A conclusion with some discussion of possible future work is presented in Ch. 5.

Chapter 2

Classical Mechanics

The Hamiltonian formulation of classical mechanics is the first example of canonical dynamics with which this work is concerned. The algebraic structure of classical dynamics provides the basic template upon which quantum dynamics is based. This structure, being present in both quantum and classical mechanics, suggests its fundamental role in physical theories.

In this chapter, the main concepts of Hamiltonian mechanics are reviewed with an emphasis on the aspects to be generalized for use in other theories, such as quantum and hybrid mechanics. The contents of this chapter use insights from [23], [24] and [25].

2.1 Poisson brackets and the dynamics of observables

In canonical classical mechanics, the basic observables come in *canonically conjugate pairs* (q, p). The pair (q, p) then forms the *canonical coordinates* of the 2-dimensional *phase space* of the system. Simple examples of conjugate pairs include the position and momentum of a point particle (x, p_x), and the angular position and angular momentum of a point particle around an axis (ϑ, p_ϑ). In general physical systems can have any number of degrees of freedom N, then the phase space is $2N$-dimensional.

The defining relations between conjugate pairs will be given in Sec. 2.1.2. For now, we just note their existence. Variables denoted q refer to the *degrees of freedom* of the system, that is, the independent ways to configure a system. A simple example

of the degrees of freedom is the (x, y, z)-position of a point particle in space. Another example is (x, y, z)-position of the center of mass of a solid body in space and the (α, β, γ)-angles (Euler angles) defining the orientation of a solid body in space. We refer to the *generalized coordinates* by q_i where i runs over any number of degrees of freedom N.

The momenta canonically conjugate to q_i are referred to as p_i. The existence of a momentum per degree of freedom is a reflection of the observational fact that two pieces of information are needed to specify the future behavior of a given degree of freedom. This fact is mathematically expressed as the equations of motion being second order in the degrees of freedom, or equivalently, as there being two first order equations, one per canonical conjugate.

The conjugate variables q and p, being observables, are represented as real numbers. This is necessary to account for the continuous nature of physical occurrences. A linear combination of the conjugate variables is also an observable. That would be the most straightforward way of constructing dynamical variables out of the basic ones. Two more interesting operations for constructing such variables will be presented in subsections 2.1.1 and 2.1.2. The structure discussed will then be used to determine the form of the dynamical evolution of observables and study symmetries.

2.1.1 The composition product

Dynamical variables $u(q, p)$ can be constructed from the basic canonical conjugate pairs via linear combination, relying on the operation of addition. Another operation used to construct more dynamical variables is the operation of ordinary multiplication.

Multiplication of two observables gives a third observable whose value can be calculated by knowledge of its factors: numerically, the value of the observable (uv) is simply the product of u and v. Measuring u and v individually would be an indirect measurement of (uv). However, in some interesting cases, one is able to measure the

composite observable (uv) directly, without measuring u and v. An example of a composite observable would be the total energy of a particle $p^2/2m + V(x)$; energy can be measured without measuring its component momentum and position.

Thus we see that multiplying dynamical variables has the potential to produce physically interesting quantities that stand on their own as observables. We shall call the product of dynamical variables a *composition product*.

For classical mechanics, normal multiplication is a composition product. An important property of this product is that it is commutative. This commutativity is connected to the classical certainty of measurement discussed in Sec. 2.3.

Another crucial property in defining a composition product is its relationship to a dynamical bracket. This property will be explained in the next subsection.

To summarize, we start with canonically conjugate pairs q and p and we are able to construct more dynamical variables as functions of them. These functions are constructed via the operations of addition and ordinary multiplication. In the next subsection, we will see yet another important operation that produces further observables.

2.1.2 The dynamical bracket

At the heart of the canonical formulation of classical mechanics lies the Poisson bracket. We start from the algebraic properties of the Poisson bracket instead of its familiar definition (2.11) to emphasize their fundamental nature, they will be present in the quantum theory in a slightly modified form. The Poisson bracket a binary operation that obeys the following axioms. For dynamical variables u, v and w, and non-dynamical scalars a and b (independent of q and p), the Poisson bracket obeys

- **Antisymmetry**

$$\{u, v\} = -\{v, u\} \ , \tag{2.1}$$

- **Scalar annihilation**

$$\{u, a\} = 0 \ , \tag{2.2}$$

- **Linearity**

$$\{u, v + w\} = \{u, v\} + \{u, w\} \ , \tag{2.3}$$

- **Leibniz rule**

$$\{u, vw\} = \{u, v\}w + v\{u, w\} \ . \tag{2.4}$$

- **Jacobi identity**

$$\{u, \{v, w\}\} = \{\{u, v\}, w\} + \{v, \{u, w\}\} \ . \tag{2.5}$$

In addition to the above axioms, canonical pairs of degrees of freedom q_i and their conjugate momenta p_i are defined through the **fundamental canonical relations**

$$\{q_i, q_j\} = 0 \ , \quad \{p_i, p_j\} = 0 \ , \quad \{q_i, p_j\} = \delta_{ij} \ , \tag{2.6}$$

where δ_{ij} is the Kronecker delta symbol and the indices i and j run from 1 to the number of independent degrees of freedom N.

Using the above setup we can define a consistent framework for dynamics. By induction, using the canonical relations and the Leibniz property of the bracket, the Poisson bracket of q_i^n with p_i is

$$\{q^n, p\} = nq^{n-1} \ . \tag{2.7}$$

Taylor expanding any dynamical variable $u(q,p)$

$$u(q,p) = \sum_{k=0}^{\infty} \frac{1}{k!} \left. \frac{\partial^k u(q,p)}{\partial q^k} \right|_{q=q_0} q^k \ , \tag{2.8}$$

and using the scalar annihilation, linearity and Leibniz properties, we find that a Poisson bracket of $u(q,p)$ with p_i is the derivative of that function with respect to q_i

$$\{u(q,p), p_i\} = \frac{\partial}{\partial q_i} u(q,p) \ . \tag{2.9}$$

We then say that *momentum* p_i is the generator of translations along the q_i. Similarly, we get

$$\{q_i, u(q,p)\} = \frac{\partial}{\partial p_i} u(q,p) \ . \tag{2.10}$$

Using the same method, plus the anitsymmetry property, we can find the Poisson bracket of any two functions of the canonical coordinates

$$\{u(q,p), v(q,p)\} = \sum_i \frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial v}{\partial q_i} \ . \tag{2.11}$$

A useful notation is to use the Poisson binary operation to symbolize the bracket as

$$\{u, v\} = u\mathcal{P}v = u\left[\sum_i \left(\overleftarrow{\partial}_{q_i}\overrightarrow{\partial}_{p_i} - \overleftarrow{\partial}_{p_i}\overrightarrow{\partial}_{q_i}\right)\right] v \ . \tag{2.12}$$

The left and right derivatives, indicated by the arrows above them, act to the left or to the right as intuitively expected, like

$$u\overleftarrow{\partial}_q v = (\partial_q u)v \ , \quad u\overrightarrow{\partial}_q v = u(\partial_q v) \ . \tag{2.13}$$

The subscript indicates the variable with respect to which the derivative is taken, like

$\partial_q = \partial/\partial q$.

The linearity and Leibniz properties of the Poisson bracket allows it to perform the role of a derivative as demonstrated by (2.9) and (2.10). This also allows the use of the bracket as a time derivative. Just as the momentum is the generator of translations along its conjugate degree of freedom, a special dynamical variable can be used as a generator of time translation. That generator is called the *Hamiltonian* $H(q, p, t)$

$$\frac{d}{dt}u = \{u, H\} + \frac{\partial u}{\partial t} \ . \tag{2.14}$$

Time is the only evolution parameter that can have a total differential operator since all dynamical variables, by definition, evolve in time. This is not to be confused with the possible explicit time dependence, captured by the partial time derivative in the dynamical evolution equation (2.14). Time evolution of any dynamical variable $u(q, p)$ (aside from explicit dependence) is a consequence of its dependence on q and p, which evolve in time according to Hamilton's equations:

$$\dot{q} = \{q, H\} \ , \qquad \dot{p} = \{p, H\} \ . \tag{2.15}$$

The dot denotes a total time derivative: $\dot{f} := df/dt$. The evolution of u due to the evolution of the canonical coordinates is called a *dynamical* evolution and is captured by the Poisson bracket $\{u, H\}$ of the variable u and the Hamiltonian H.

A variable u whose Poisson bracket with the Hamiltonian vanishes ($\{u, H\} = 0$) does not evolve dynamically. It does not change with the motion of the canonical coordinates. We call this variable a *constant of motion*. If it has no time dependence either, then it is a conserved quantity.

An explicit time dependence for an observable implies that it is interacting with other dynamical variables that were not included in the set of canonical coordinates

under consideration. No explicit time dependence should appear (outside of the canonical coordinates) if the system is closed.

The change of the Hamiltonian with respect to time is given by

$$\frac{dH}{dt} = \{H, H\} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t} \ , \tag{2.16}$$

showing that the only time dependence a Hamiltonian can have is explicit. The generator of dynamical evolution does not, itself, evolve dynamically.

A time-dependent Hamiltonian is still used to generate time transformations. These transformations will be themselves time dependent. A time-dependent Hamiltonian is not conserved.

The special role of the Hamiltonian does not imply that it is special as a function of the canonical coordinates. The Hamiltonian is an observable that is constructed as a function of the canonical coordinates; any such function is not different, in character, from any other. It is the dependence of the equations of motion on the form of the Hamiltonian that gives it its special role.

Since it specifies the equations of motion, a Hamiltonian is a complete description of the dynamics of a given physical system. A familiar example of a Hamiltonian is

$$H = \frac{p^2}{2m} + V(q) \ , \tag{2.17}$$

where m is the mass of a point particle and $V(q)$ is a potential energy function that defines a conservative force $F = -\partial V/\partial q$. The Hamiltonian equations of motion (2.15) then give

$$\dot{q} = \frac{p}{m} \ , \quad \dot{p} = -\frac{\partial V(q)}{\partial q} \quad \Rightarrow \quad F(q) = m\ddot{q} \ . \tag{2.18}$$

Different systems are described by different potentials: the simple harmonic oscillator

has $V \sim q^2$, Newtonian gravity has $V \sim 1/q$, etc. Determining the Hamiltonian describing a given system is not a question of dynamics. For that, a theory of interactions is needed, possibly based on arguments of symmetry.

2.1.3 Canonical transformations

The dynamical setup depends crucially on the canonical relations (2.6). These relations must be guaranteed to exist after the system has gone through some transformation. This transformation could be translation, rotation, dynamical evolution or a coordinate transformation to give a few examples.

Let γ parameterize some transformation of the dynamical variables. Then the value of the variable after transformation is given in terms of the value before transformation through a Taylor expansion

$$u(\gamma) = e^{\gamma \frac{\partial}{\partial \gamma}} u(0) \ . \tag{2.19}$$

The notation used above is

$$e^{\gamma \frac{\partial}{\partial \gamma}} u(0) := \left[\sum_{k=0}^{\infty} \frac{1}{k!} \gamma \frac{\partial^k u(\gamma')}{\partial \gamma'^k} \right]_{\gamma'=0} \ . \tag{2.20}$$

If the transformation is generated by a dynamical variable G (like p for q-translation or H for t-translation), then we define the operator

$$\{\cdot, G\} \ u := \{u, G\} \tag{2.21}$$

and the transformation equation (2.19) becomes

$$u(\gamma) = e^{\gamma \{\cdot, G\}} u(0) \ . \tag{2.22}$$

A *canonical transformation* is a special kind of transformation that preserves the

canonical structure, that is, it leaves the fundamental canonical relations (2.6) unchanged. If any dynamical variable u transforms as $u \to u' = e^{\gamma \frac{\partial}{\partial \gamma}} u$ then a canonical transformation $\{q, p\} \to \{q, p\}'$ is one such that $\{q, p\}' = \{q', p'\}$.

The Jacobi identity (2.5) plays a central role in ensuring that the fundamental canonical relations retain their form after transformation. To see that, consider the transformation generated by the dynamical variable G, then

$$\frac{\partial}{\partial \gamma} q = \{q, G\} \ , \quad \frac{\partial}{\partial \gamma} p = \{p, G\} \ , \quad \frac{\partial}{\partial \gamma} \{q, p\} = \{\{q, p\}, G\} \ . \tag{2.23}$$

Now expanding $\{q, p\}' = e^{\gamma \frac{\partial}{\partial \gamma}} \{q, p\}$ and $\{q', p'\} = \{e^{\gamma \frac{\partial}{\partial \gamma}} q, e^{\gamma \frac{\partial}{\partial \gamma}} p\}$, we see that

$$\{q, p\}' = \{q, p\} + \gamma \{\{q, p\}, G\} + \mathcal{O}(\gamma^2) \ , \tag{2.24a}$$

$$\{q', p'\} = \{q, p\} + \gamma \left(\{q, \{p, G\}\} + \{\{q, G\}, p\} \right) + \mathcal{O}(\gamma^2) \ . \tag{2.24b}$$

The notation $\mathcal{O}(x^n)$ is a shorthand for terms of order x^m, for all $m \geq n$. The Jacobi identity is exactly the equality of the terms in the first order of the expansion. This is all we need to show that this kind of transformation leaves the basic dynamical framework invariant. This is not surprising, the whole apparatus was constructed to do just that.

An important property of canonical transformations is that they preserve "volumes" in phase space: the Jacobian determinant $|J|$ is 1. We can prove this in a 2-dimensional phase space, the result is easily generalized to $2N$ dimensions. First, we start with a general result. Let F and G be functions of (q, p) and let γ be the

parameter of the transformation generated by G. Then we have

$$\{F, G\} = \frac{\partial F}{\partial \gamma} \tag{2.25}$$

$$= \frac{\partial F}{\partial q}\frac{\partial q}{\partial \gamma} + \frac{\partial F}{\partial p}\frac{\partial p}{\partial \gamma} \tag{2.26}$$

$$= \{F, p\}\{q, G\} - \{q, F\}\{G, p\} \ . \tag{2.27}$$

Now we turn to the Jacobian determinant. We see that

$$|J| = \frac{\partial q'}{\partial q}\frac{\partial p'}{\partial p} - \frac{\partial p'}{\partial q}\frac{\partial q'}{\partial p} \tag{2.28}$$

$$= \{q', p\}\{q, p'\} - \{q, q'\}\{p', p\} \tag{2.29}$$

$$= \{q', p'\} \ . \tag{2.30}$$

Since canonical transformations preserve the canonical relations, we have $\{q', p'\} = 1$, thus $|J| = 1$ implying that volumes in phase space are invariant under canonical transformations.

The above result allows us to picture canonical transformations as a flow of an incompressible fluid of phase space points. That is one statement of *Liouville's theorem*. We shall return to this point later in section 2.2.

2.1.4 Symmetries

Symmetry principles are at the heart of physical theories. Indeed, defining a dynamical framework in Sec. 2.1.2 was based on a certain symmetry, that of the framework itself. The *theory* should not change from one observer to another. Familiar examples of symmetry principles include the principle of relativity: the laws of physics are the same for all inertial observers, and principles of gauge invariance in electrodynamics: the field equations are same for all gauge choices.

A symmetry arises when a transformation that leaves some aspect of the system

unchanged. Allowed transformations are the ones built from the dynamical bracket, as discussed earlier in the section. If G is a dynamical variable that generates a transformation, and if u is a dynamical variable that remains unchanged with the transformation, then their Poisson bracket vanishes

$$\{u, G\} = 0 \ . \tag{2.31}$$

We say that G generates a symmetry of u. If γ is the parameter then we say that a transformation along γ is a symmetry of u.

Since any observable can generate a transformation, then if G generates a symmetry of u, the relation can be inverted (thanks to the antisymmetry of the Poisson bracket) to read u, equivalently, generates a symmetry of G.

The special role of Hamiltonian as the generator of time translation and encoder of a system's dynamics is reflected in a special relationship between symmetries of the *system* and conservation laws. Consider a dynamical variable G that generates a symmetry of the Hamiltonian

$$\{H, G\} = 0 \ . \tag{2.32}$$

Since the Hamiltonian specifies a system, then the above relation means that the system (or its equation of motion) is invariant under the symmetry generated by G. This directly implies that the Hamiltonian is independent of the transformation parameter γ

$$\frac{\partial H}{\partial \gamma} = 0 \ . \tag{2.33}$$

Now the relation $\{H, G\} = 0$ can be reversed to be

$$\{G, H\} = 0 \ , \tag{2.34}$$

meaning that G is a constant of motion. If G does not have an explicit time dependence, then from the equation of motion for $\dot{G} = \{G, H\} + \partial G/\partial t$ we see that G is a conserved quantity. We thus arrive at *Noether's theorem: for every continuous symmetry of the system there exists a conserved quantity.* We see that the theorem takes a particularly simple form in the Hamiltonian formulation.

An example would be translation along the x-axis, that is a transformation generated by the momentum p_x. If the dynamics of the system doesn't change along the x-axis then $\{H, p_x\} = \partial H/\partial x = 0$, and p_x is conserved.

Conservation laws are important. Their existence and relationship to symmetry derive from the existence of a consistent dynamical bracket.

2.2 Classical states

Mechanics is concerned with the prediction of future behaviour of a system based on current knowledge of it. The state of the system is the information needed at a given instant of time in order to calculate the same information at a later time. This information then constitutes the description of the system.

In the previous section, we have seen the algebra of the dynamical bracket and observables. In this section, we will discuss the construction of the state of a system and how to extract measurable information from it. This topic is fairly straightforward in classical mechanics. Nonetheless, we discuss it in anticipation of the corresponding treatment in quantum mechanics.

2.2.1 States of complete and partial knowledge

In the setup we have constructed thus far, we are interested in dynamical variables that are functions of the canonical coordinate $u(q,p)$. Knowledge of the canonical coordinates as functions of time, then, is enough to describe the system. To find this time dependence, we need to solve the $2N$ first-order Hamiltonian equations of motion

$$\dot{q} = \{q, H\} \ , \quad \dot{p} = \{p, H\} \ . \tag{2.35}$$

Arriving at the solution requires the knowledge of $2N$ values of the (q,p) at an instant of time. Each such set of $2N$ values specifies a state of the system, and the collection of such points is the space of states.

In practice, a complete knowledge of the degrees of freedom and their momenta is not always available. A large number of particles would be difficult to measure individually, for example, or even for a few particles we could simply have limited precision of the measuring device. We then have access only to a partial knowledge of the system. If this same partial knowledge can be calculated, using the equations of motion, for different instants of time, then it constitutes a state of the system as well.

The natural representation of the knowledge of phase space variables (q,p) would be a probability distribution. If complete knowledge is unavailable, the best we can have for measurable predictions are expectation values of dynamical variables. These can be calculated using the probability distribution ρ obeying the constraints

$$\rho \geq 0 \ , \quad \int_{-\infty}^{\infty} dq\, dp\ \rho = 1 \ . \tag{2.36}$$

From now on, the explicit limits of integration will be dropped and all integrals are understood to be over all possible values of q and p. Initially (at $t = 0$), the expectation

value of a dynamical variable u is given by

$$\langle u\rangle(0) = \int dq_0\, dp_0\ \rho(q_0,p_0)u(q_0,p_0)\ , \tag{2.37}$$

where (q_0, p_0) are the phase space coordinates at $t = 0$.

The expectation value of a dynamical variable should evolve in time according to the evolution of the canonical coordinates. Let us consider only time-independent Hamiltonians, then following the discussion in the previous section we have

$$u(t) = u\big(q(t),p(t)\big) = e^{t\{\cdot,H\}}u(q_0,p_0) = e^{t\{\cdot,H\}}u(0)\ . \tag{2.38}$$

Then the expectation value at a later time is given by

$$\langle u\rangle(t) = \int dq_0\, dp_0\ \rho(q_0,p_0)\left(e^{t\{\cdot,H\}}u(q_0,p_0)\right)\ . \tag{2.39}$$

The uncertainty in the value of u at a later time is a result of the uncertainty in the values of q and p initially.

With (q_0, p_0) denoting all phase space points at an initial instant, a state of complete knowledge would have a Dirac delta function $\delta(q_i - q_0, p_i - p_0)$ as its probability distribution, where (q_i, p_i) are the exact initial canonical coordinates. A partial, or incomplete knowledge of the system would be described by any other distribution. We call the distribution ρ a *state distribution*.

It is important to note that determining the state distribution is not a question of dynamics. The state distribution represents our knowledge of the system. Dynamics is then applied to this information.

2.2.2 Dynamical evolution of the state

The description of mechanics presented thus far views the canonical phase space coordinates as functions of time. All other dynamical variables have an implicit time

dependence due to their functional dependence on the canonical coordinates. This view is natural when complete knowledge of the system is present. Indeed, it is common to call the set of these coordinates the state of the system and its evolution is simply the equation of motion of the canonical coordinates. This view of dynamics is called the *Heisenberg picture*[1].

For an incomplete knowledge of the initial values (q_0, p_0), the calculation of expectation values of dynamical variables using the expression (2.39) can be cumbersome. It requires solving $2N$ equations of motion for the canonical variables. A different point of view can make the calculation simpler.

In the Heisenberg picture, our knowledge of the system is embodied in the knowledge of the initial state of the system. We can, alternatively, think of this state as evolving with time to reflect the change in our knowledge of the system over time. This picture will require that we treat the canonical coordinates as unchanging in time. Instead, it is the probability of the system acquiring a particular value at a certain point in phase space that evolves in time. This is the *Schrödinger picture*[2].

The equivalence between these two pictures hinges on the description of time evolution as a canonical transformation. We now show how this equivalence can be demonstrated. First we see that the integral of any two functions on phase space is invariant under canonical transformation $f(q,p) \to f'(q,p) = e^{\gamma\{\cdot,G\}} f(q,p) = f(q',p')$

$$\int dq\, dp\ f(q',p')\ g(q',p') = \int |J|\ dq' dp'\ f(q',p')\ g(q',p') \tag{2.40}$$

$$= \int dq\, dp\ f(q,p)\ g(q,p)\ . \tag{2.41}$$

It is the property of canonical transformations having a unit Jacobian determinant $|J|$ that allows this equality. Now, since time evolution is a canonical transformation, applying this, with $\gamma = -t$ and $G = H$, to the expectation value equation (2.39), we

[1] The term is borrowed from quantum mechanics.
[2] Check the previous footnote.

get

$$\langle u \rangle(t) = \int dq_0\, dp_0 \left(e^{-t\{\cdot, H\}} \rho(q_0, p_0) \right) u(q_0, p_0) \ . \tag{2.42}$$

Of course, the integration variables can be renamed, but we leave them in this form to emphasize their relationship to $\big(q(0), p(0)\big)$ in the Heisenberg picture. The phase space coordinates are fixed.

The state distribution can now be viewed as an explicit function of time that evolves according to

$$\rho(q_0, p_0; t) = e^{-t\{\cdot, H\}} \rho(q_0, p_0; 0) \ . \tag{2.43}$$

Notice the minus sign. The two pictures now appear merely as opposing points of view. The Heisenberg picture is one of dynamic variables moving on a fixed background of a probability distribution; the Schrödinger picture is one of a state distribution flowing on a fixed coordinate system.

Equation (2.43) can be rewritten as

$$\frac{\partial \rho}{\partial t} = -\{\rho, H\} \ . \tag{2.44}$$

This is the Liouville equation governing the evolution of the state. It can further be rewritten as

$$\frac{d\rho}{dt} = \{\rho, H\} + \frac{\partial \rho}{\partial t} = 0 \ . \tag{2.45}$$

This form gives the state distribution the appearance of a special case of a dynamical variable. It is yet another manifestation of the incompressible flow in phase space described by canonical transformations.

If we define position vectors in the $2n$-dimensional phase space as

$$\mathbf{x} := (q_1, \cdots, q_n, p_1, \cdots, p_n) = (x_1, \cdots, x_{2n}) \ , \tag{2.46}$$

then, using Hamilton's equations $\dot{\mathbf{x}} = \{\mathbf{x}, H\}$, the Liouville equation takes the form of a continuity equation

$$\nabla \cdot (\rho \, \dot{\mathbf{x}}) + \frac{\partial \rho}{\partial t} = 0 \tag{2.47}$$

with $\rho \dot{\mathbf{x}}$ acting as the flux of the probability current. This ensures that the role of the state distribution as a probability distribution is preserved over time. If the state distribution is initially nonnegative and normalized, then it remains so for all times.

2.3 Classical measurement and determinism

Earlier, it was claimed that determining the state distribution is not a question of dynamics. Dynamics is what happens after a state is determined. How, then, is a state determined? An act of measurement is a form of interaction between a measuring device and the system under consideration. Thus, dynamics is involved. Moreover, an interaction, by virtue of being an "inter"-"action" inevitably introduce some disturbance to the system being measured.

Classical experience of the world shows that the uncertainty in the future behaviour of systems can be reduced by more precise measurements of the initial state. It is this experience that motivates postulating an extreme extension of it: *measurements can be made indefinitely weak*. That is, it is a matter of technology to invent more precise devices that introduce less disturbance to the measured system. It also has to be postulated that the initial state of the measuring device, itself a physical system, is perfectly known.

The uncertainty in the value of a dynamical variable u is given by

$$\Delta u = \sqrt{\langle (u - \langle u \rangle)^2 \rangle} \ , \tag{2.48}$$

where $\langle u \rangle$ is the expectation value of u. The postulate that the state can be completely known translates into the state distribution being a Dirac delta function giving a vanishing uncertainty

$$\langle u \rangle = u \Rightarrow \Delta u = 0 \ . \tag{2.49}$$

This conforms with the classical experience of measurement. Infinite precision implies determinism.

There is more to this story. In Sec. 3.4 we will see that the choice of a noncommutative composition product for dynamics will necessarily exclude the possibility of infinitely precise measurements of phase space variables. This will come at a cost.

Chapter 3

Quantum Mechanics

Quantum mechanics is the framework needed to describe phenomena at the small scale that cannot be accounted for by classical mechanics. Two key properties of these phenomena are *uncertainty* and *nonlocality*. The former is the fundamental limit to the precision with which we can simultaneously measure certain pairs of variables. The latter is the dependence of the outcome of measurement at one point in space on the physical setup at another, distant point.

Heisenberg's uncertainty principle quantifies the limit of precision of simultaneous measurements of, for example, canonical pairs of variables as

$$\Delta q \, \Delta p \geq \frac{\hbar}{2} \, . \tag{3.1}$$

Planck's constant, $\hbar$, defines a minimum area in the phase space of q and p. This inequality reflects that the more certain the measurement of q is, the more uncertain is the measurement of p.

The nonlocality property of quantum mechanics is apparent in the phenomenon of entanglement. The outcome of measurement at one point in space may depend on the outcome of a measrement at a distant point. A key feature in our current understanding of quantum nonlocality is that it is not interaction-based. Rather, it is a built-in correlation between distant physical objects.

In this chapter we will see how these two features (uncertainty and nonlocality) can be integrated into the same basic structure of the dynamical framework discussed

in the previous chapter. For the most part, we will be using the phase space quantum mechanics. Readers interested in learning more about this formulation can find extensive resources in [26, 27, 28, 29, 30, 31, 32, 33, 34, 35], or more pedagogical reviews in [36, 37, 38, 39].

3.1 Commutator brackets and the dynamics of observables

Even though quantum mechanics deals with phenomena so foreign to our immediate senses, we can still perform different kinds of measurements. Thus quantum mechanics, just like classical mechanics, has observables. Observables, and dynamical variables in general, undergo change, or transformation. This time, instead of the classical Poisson bracket $\{\cdot, G\}$ being the operator enforcing the transformation, we introduce the quantum dynamical bracket $[\![\cdot, G]\!]$. The transformation, just like the one discussed in the classical case, if continuous, can be described as

$$u(\gamma) = e^{\gamma[\![\cdot, G]\!]} \ . \tag{3.2}$$

Here, again, γ is a transformation parameter and G is a dynamical variable that generates this transformation.

The physical requirements of the previous chapter are still in force. This will lead to the same algebraic structure of classical dynamical brackets. However, one feature of classical mechanics that was not motivated by a strong physical requirement is its composition product. In this section we will see how choosing a suitable composition product for quantum mechanics will give rise to a framework capable of describing quantum phenomena.

3.1.1 The composition product

As discussed in Sec. 2.1.1, a composition product has to form a group with the set of dynamical variables as its elements. The composition product used for classical

mechanics is ordinary (pointwise) multiplication, which is commutative. The commutativity of a composition product is an extra condition that was not necessitated by any of the physical conditions discussed.

In general, composition products can be noncommutative. The commutator of a noncommutative, linear and associative product naturally provides a candidate for the dynamical bracket. The commutator is a Lie bracket that identically obeys the Leibniz rule with respect to the composition product. This will be detailed in Sec. 3.1.2. If the composition product is nonlocal, then its commutator can, in general, be nonlocal as well. If that commutator is used as the dynamical bracket, then nonlocality can be implemented in the dynamics. Further, as we will see in Sec. 3.4.1, a noncommutative composition product will give rise to uncertainty relations like that of Heisenberg.

Let us consider a nonlocal, noncommutative composition product for quantum mechanics. We call it a *star product* ($\star$-product). New dynamical variables can be constructed from known variables by linear combinations and applying the composition product. This requires that the $\star$ product reduces to normal multiplication when acting on a nondynamical variable, or a scalar a

$$u \star a = a \star u = a\, u \ . \tag{3.3}$$

The discussion so far does not fix this product. Indeed, fixing this product is no simple task. But one more condition needs to be imposed that should define the relationship between quantum and classical dynamics.

Classical mechanics is very successful in describing the phenomena of our everyday experience. But the objects of this experience are made of molecules and atoms, objects that obey quantum mechanics. Thus, in constructing quantum mechanics, we must make it such that it can give rise to classical mechanics in some limit. That is the subject of section 3.3. For now, we use this to impose two conditions. The first is that we use the mathematical entities to describe dynamical variables in quantum

mechanics as those we used for classical mechanics. The second condition is that the quantum composition should reduce to the classical one in the appropriate limit

$$\star = 1 + \mathcal{O}(\hbar) \ . \tag{3.4}$$

We see that

$$\lim_{\hbar \to 0} u \star v = u\, v \ . \tag{3.5}$$

The *deformation parameter* $\hbar$ thus measures the deviation from classicality into quantumness. Along with noncommutativity, associativity and linearity, condition (3.4) defines the general properties of a $\star$-product.

The expansion of the $\star$-product in powers of the deformation parameter $\hbar$ is not unique. We shall not address this nonuniqueness at the moment. Formally, we represent this expansion as [32]

$$\star = 1 + \sum_{n=1}^{\infty} (i\hbar)^n \mathcal{G}_n \ . \tag{3.6}$$

The products (binary operations) $\mathcal{G}_n$ encode the noncommutativity of the $\star$-product and $i = \sqrt{-1}$ is the imaginary unit. Here we are using a similar notation to that used in defining the Poisson product $\mathcal{P}$ in (2.12). Equation (3.6) should imply

$$u \star v = uv + \sum_{n=1}^{\infty} (i\hbar)^n \, u \, \mathcal{G}_n v \ . \tag{3.7}$$

A more familiar notation in the literature is

$$u \star v = uv + \sum_{n=1}^{\infty} (i\hbar)^n \, \mathcal{G}_n(u, v) \ . \tag{3.8}$$

We prefer to use the notation $u \, \mathcal{G}_n v := \mathcal{G}_n(u, v)$ because it allows for a less cumbersome

analysis of the properties of $\mathcal{G}_n$ as a product. The linearity of $\star$ implies the linearity of the $\mathcal{G}_n$.

The associativity of $\star$, when expanded

$$(u \star v) \star w = u \star (v \star w) \tag{3.9}$$

$$[u\,(1 + i\hbar\mathcal{G}_1 + \cdots)\,v]\,(1 + i\hbar\mathcal{G}_1 + \cdots)\,w = u\,(1 + i\hbar\mathcal{G}_1 + \cdots)\,[v\,(1 + i\hbar\mathcal{G}_1 + \cdots)\,w] \tag{3.10}$$

gives the relation

$$(uv)\mathcal{G}_1 w + (u\mathcal{G}_1 v)w = u(v\mathcal{G}_1 w) + u\mathcal{G}_1(vw)\ . \tag{3.11}$$

This relates the first-order expansion of the $\star$ product and normal multiplication. This condition would be satisfied identically if $\mathcal{G}_1$ obeys the Leibniz rule with respect to normal product $u\mathcal{G}_1(vw) = (u\mathcal{G}_1 v)w + v(u\mathcal{G}_1 w)$. The importance of $\mathcal{G}_1$ will be shown in the next subsection.

The nonuniqueness of the $\star$-product, mentioned earlier, is a reflection of the nonuniqueness of the deformation of classical mechanics into quantum mechanics. There are multiple ways to generalize classical mechanics into quantum mechanics. Those deformations are connected, among other things, to operator ordering schemes in operator quantum mechanics as will be discussed in Sec 3.2. Formally, different $\star$-products will satisfy the same general criteria if they preserve the same algebra, that is, if they are related by a *transition operator* in a homomorphism [32]

$$T(A \star B) = (TA) \star' (TB)\ . \tag{3.12}$$

Here, A and B are arbitrary dynamical variables (elements of the algebra) and T is

the transition operator that can be expanded formally as

$$T = 1 + \sum_{n}^{\infty} (i\hbar)^n T_n \ , \tag{3.13}$$

where T_n are linear operators. $\star$-products related in such way are called *c-equivalent* (cohomologically equivalent) [34].

The products $\mathcal{G}_n$ are generally bidifferential operators (see [40]), and their infinite sum implies the nonlocality of the $\star$-product. The nonlocality of the $\star$-product is apparent in its integral form in the Wigner representation [33]

$$u \star_W v \propto \int dx'dp'dx''dp'' f(x+x', p+p')\, g(x+x'', p+p'')\, e^{-\frac{2}{i\hbar}(x'p''-x''p')} \ . \tag{3.14}$$

Since $\star$-products are related to each other via the transition operator (3.13), the nonlocality expressed for the Wigner $\star_W$-product implies the nonlocality for any $\star$-product.

3.1.2 The dynamical bracket

We now show that the commutator of the $\star$-product is a natural candidate for a dynamical bracket fitting the needs of quantum mechanics. The $\star$-commutator is defined as

$$[\cdot\,,\cdot] := \star - \star^t \ . \tag{3.15}$$

The superscript t signifies the transpose of the product, the product taken in the reverse order: $u \star^t v = v \star u$. Then the equation above is

$$[u, v] = u \star v - u \star^t v = u \star v - v \star u \ . \tag{3.16}$$

The commutator of a noncommutative, linear and associative product is identically antisymmetric, linear and obeys the Jacobi identity

$$[u, v] = -[v, u] \ , \tag{3.17}$$

$$[u, av + bw] = a[u, v] + b[u + w] \ , \tag{3.18}$$

$$[u, [v, w]] = [[u, v], w] + [v, [u, w]] \ , \tag{3.19}$$

making it a Lie bracket. It is also an identity that the commutator of a linear and associative product obeys the Leibniz rule with respect to that product

$$[u, v \star w] = [u, v] \star w + v \star [u, w] \ . \tag{3.20}$$

Thus, $[\cdot\,,\cdot]$ fulfills the requirements of a dynamical bracket if $\star$ is the composition product.

Now we use the argument that classical dynamics must emerge from quantum dynamics in some limit to impose an extra condition on the commutator and, consequently, on the $\star$-product. The quantum dynamical bracket must reduce to the classical dynamical bracket in the same limit that reduces the quantum $\star$-product to the classical normal multiplication.

Expanding the commutator in powers of $\hbar$ we get

$$[\cdot\,,\cdot] = \sum_{n=1}^{\infty} (i\hbar)^n (\mathcal{G}_n - \mathcal{G}_n^t) \ . \tag{3.21}$$

Since the products $\mathcal{G}_n$ do not contain $\hbar$, we see that the commutator vanishes in the limit $\hbar \to 0$. We may define the dynamical bracket $[\![\cdot\,,\cdot]\!]$ as

$$[\![\cdot\,,\cdot]\!] := \frac{1}{i\hbar}[\cdot\,,\cdot] \ . \tag{3.22}$$

Now we can have

$$\lim_{\hbar\to 0}[\![\cdot\,,\cdot]\!] = \{\cdot\,,\cdot\}\ , \tag{3.23}$$

giving us the condition

$$\mathcal{G}_1 - \mathcal{G}_1^t = \{\cdot\,,\cdot\}\ . \tag{3.24}$$

That is, the Poisson bracket is the commutator of the $\mathcal{G}_1$-product. Thus, $\mathcal{G}_1$ must be noncommutative.

Being noncommutative, the product $\mathcal{G}_1$ can be further split into symmetric and antisymmetric parts, with the antisymmetric part being the Poisson bracket

$$\mathcal{G}_1 = \frac{1}{2}(\mathcal{P} + \sigma)\ . \tag{3.25}$$

We have used the notation $\mathcal{P}$ for the Poisson bracket introduced in Ch. 2. The symmetric part, σ, is defined as

$$\sigma := \mathcal{G}_1 + \mathcal{G}_1^t\ . \tag{3.26}$$

The nonuniqueness of $\star$ implies the nonuniqueness of $\mathcal{G}_1$. The symmetric part, σ, can differ, but the antisymmetric part is fixed to be the Poisson bracket $\mathcal{P}$. It is the relationship between $\mathcal{G}_1$ and the classical dynamical bracket $\mathcal{P}$ that makes $\mathcal{G}_1$ important for the current work.

Similar to the classical fundamental canonical relations, the quantum fundamental canonical relations are given in terms of the quantum dynamical bracket

$$[\![q_i, q_j]\!] = 0\ , \quad [\![p_i, p_j]\!] = 0\ , \quad [\![q_i, p_j]\!] = \delta_{ij}\ . \tag{3.27}$$

The momentum p canonically conjugate to q generates transformations parametrized by q, as discussed in Ch. 2. Thus, if a dynamical variable f is a function of (q,p) constructed using addition, scalar multiplication and the $\star$-product, then we have

$$[\![q,f]\!] = \frac{\partial f}{\partial p} \ , \quad [\![f,p]\!] = \frac{\partial f}{\partial q} \ . \tag{3.28}$$

These relations can be proven using the algebraic properties of $[\![\cdot\,,\cdot]\!]$. In general, if G is the generator of transformations parametrized by γ then

$$[\![f,G]\!] = \frac{\partial f}{\partial \gamma} \ . \tag{3.29}$$

The observable that generates time translations for the system is the Hamiltonian H. Following the same argument in Ch. 2, the time evolution of a dynamical variable f is given by

$$\frac{df}{dt} = [\![f,H]\!] + \frac{\partial f}{\partial t} \ . \tag{3.30}$$

This is the equation of motion in the Heisenberg picture. And, again, same as in the previous chapter, an observable G is conserved if it generates a symmetry of the Hamiltonian

$$[\![H,G]\!] = 0 \ , \quad [\![G,H]\!] = 0 \ . \tag{3.31}$$

We see from the discussion in this section that the formal structure of the dynamical framework of both quantum and classical and quantum mechanics is more or less unified. This unity is apparent in the Hamiltonian formulation in phase space. The differences lie in the composition product.

3.2 Quantum state distributions

Unlike classical mechanics, quantum mechanics is a theory where simultaneous measurements of canonically conjugate variables are limited by Heisenberg's uncertainty principle. There is a fundamental restriction on the available knowledge that we can obtain from measurement. This implies that the concept of a state is indispensable in quantum mechanics.

Up to this point, we have discussed mechanics, classical or quantum, purely in terms of phase space notions. However, now we have reached a point where, in order to derive key properties of the quantum state distribution, it would be easier to resort to the older, more familiar, formulation of quantum mechanics. Here we present a brief overview of operator quantum mechanics before returning to the phase space formulation.

Operator quantum mechanics describes systems in terms of state vectors $|\psi\rangle$ in Hilbert space. Dynamical variables $\hat{A}$ are represented as operators acting on the vectors of this space. The expectation value of a dynamical variable is given by

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle \ . \tag{3.32}$$

The state could also be described in terms of a state operator $\hat{\rho}$

$$\hat{\rho} = \sum_i \omega_i |\psi_i\rangle\langle\psi_i| \tag{3.33}$$

where ω_i are nonnegative numbers obeying $\sum_i \omega_i = 1$. They represent the probability that the system is in state $|\psi_i\rangle$. A pure state is described by a state operator where all but one of the ω_i vanish

$$\hat{\rho} = |\psi\rangle\langle\psi| \ . \tag{3.34}$$

Otherwise, $\hat{\rho}$ describes a general or a mixed state; one that is a mixture of pure states. The state operator obeys the following conditions

$$\mathrm{Tr}(\hat{\rho}) = 1 \ , \quad \hat{\rho}^{\dagger} = \hat{\rho} \ , \quad \langle \phi | \hat{\rho} | \phi \rangle \geq 0 \ , \tag{3.35}$$

where $|\phi\rangle$ is a general state. These conditions allow us to calculate expectation values in terms of the state operator as

$$\langle \hat{A} \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}) \ . \tag{3.36}$$

In addition to conditions (3.35), a pure state operator must also obey

$$\hat{\rho}^2 = \hat{\rho} \ . \tag{3.37}$$

That is, a pure state operator is idempotent.

Of relevance to the current work is the state operator description of a system made up of two parts. Let $\hat{\rho}$ be the state operator of the entirety of systems (1) and (2), then taking a partial trace of $\hat{\rho}$ with respect to (2) and (1), respectively, yields

$$\hat{\rho}_1 = \mathrm{Tr}_2(\hat{\rho}) \ , \qquad \hat{\rho}_2 = \mathrm{Tr}_1(\hat{\rho}) \ . \tag{3.38}$$

It is evident from $\mathrm{Tr}(\hat{\rho}) = 1$ that

$$\mathrm{Tr}_1(\hat{\rho}_1) = 1 \ , \qquad \mathrm{Tr}_2(\hat{\rho}_2) = 1 \ . \tag{3.39}$$

Further, it can be shown that $\hat{\rho}_1$ and $\hat{\rho}_2$ satisfy the conditions (3.35) for state operators. Now we can see that, similar to (3.36), the expectation value of an operator A_1

belonging only to system (1) can be given in terms of $\hat{\rho}_1$ only

$$\langle \hat{A}_1 \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}_1) = \mathrm{Tr}_1\big(\mathrm{Tr}_2(\hat{\rho}\hat{A}_1)\big) = \mathrm{Tr}_1\big(\hat{\rho}_1\hat{A}_1\big) \ . \tag{3.40}$$

That is, $\hat{\rho}_1$ is a state operator for system (1) and, similarly, $\hat{\rho}_2$ for system (2). However, in general, we have

$$\hat{\rho}_1^2 \neq \hat{\rho}_1 \ , \tag{3.41}$$

and similarly for $\hat{\rho}_2$. In general, subsystems (1) and (2) are in a mixed state even if the full system is in a pure state. The subsystems are guaranteed to be pure only if the full system is comprised of two noninteracting subsystems that are both pure. Thus, for interacting systems, they are, in general, described by a mixed state operator.

Time evolution in operator quantum mechanics can be described through the Heisenberg picture, where the state contains information about the initial conditions only, while the dynamical operators evolve in time according to the Heisenberg equation

$$\frac{d\hat{A}}{dt} = \frac{1}{i\hbar}(\hat{A}\hat{H} - \hat{H}\hat{A}) + \frac{\partial \hat{A}}{\partial t} \ . \tag{3.42}$$

Equivalently, in the Schrödinger picture, dynamical operators can be viewed as fixed in time while the state evolves according to the von Neumann equation

$$\frac{1}{i\hbar}(\hat{\rho}\hat{H} - \hat{H}\hat{\rho}) + \frac{\partial \hat{\rho}}{\partial t} = 0 \ , \tag{3.43}$$

which is equivalent to the Schrödinger equations. For a nice discussion of the equation for state operator in the Schrödinger and Heisenberg pictures, see [25].

Let $\hat{\rho}$ be the state operator of a system whose Hamiltonian is $\hat{H}$. Further, let $\hat{\rho}$ be a simple tensor product $\hat{\rho}_1 \otimes \hat{\rho}_2$ of the state operators of two subsystems. We see

that if the Hamiltonian contains no interaction terms between subsystems (1) and (2), then $\hat{\rho}_1$ and $\hat{\rho}_2$ will obey the von Neumann equation. If $\hat{\rho}$ is not a tensor product, or if the two subsystems interact, then $\hat{\rho}_1$ and $\hat{\rho}_2$ do not, in general, follow the von Neumann evolution [41].

Now we translate operator quantum mechanics into the phase space language where (3.35) will give us clear conditions on the quantity that can be used as a quantum state distribution.

A quantization map

$$\mathcal{Q} : f \mapsto \hat{f} \tag{3.44}$$

is used to construct Hilbert space operators representing quantum dynamical variables from their corresponding classical phase space functions

$$q \to \hat{q} = \mathcal{Q}(q) \ , \quad p \to \hat{p} = \mathcal{Q}(p) \ , \tag{3.45}$$

$$f(q,p) \to \hat{f}(\hat{q},\hat{p}) = \mathcal{Q}(f) \ . \tag{3.46}$$

One can construct phase space functions corresponding to Hilbert space operators via a *dequantization* map

$$\mathcal{Q}^{-1}(\hat{f}) = f \ , \tag{3.47}$$

where $\hat{f}$ is the operator and f is the *symbol* corresponding to it. Just as the quantization map is not unique (for example, due to the operator ordering ambiguity), the dequantization is not, either.

The algebra of operators and their product is mimicked by the algebra of functions

and the $\star$-product. A given dequantization map acting on product of operators yields

$$\mathcal{Q}^{-1}(\hat{f}\hat{g}) = f \star g \ , \tag{3.48}$$

$$\mathcal{Q}^{-1}\left(\frac{1}{i\hbar}(\hat{f}\hat{g} - \hat{g}\hat{f})\right) = [\![f, g]\!] \ . \tag{3.49}$$

Now that the basic elements of the operator language have been translated into phase space, we move on to define suitable state distributions on phase space.

The most famous phase space representation of quantum mechanics is the Wigner distribution accompanied by its corresponding $\star$-product. In that representation, the symbol A_W for the operator $\hat{A}$ is obtained through the Wigner transform

$$A_W = \int dq' \, e^{ipq'/\hbar} \left\langle q - \frac{1}{2}q' \middle| \hat{A} \middle| q + \frac{1}{2}q' \right\rangle \ . \tag{3.50}$$

It is the inverse of the Weyl quantization map thus reflecting the Weyl operator ordering scheme

$$\mathcal{Q}_{\text{Weyl}}\left(e^{aq+bp}\right) = e^{a\hat{q}+b\hat{p}} \ , \tag{3.51}$$

where a and b are arbitrary constants. The $\star$-product corresponding to this representation is

$$\star_W = e^{\frac{i\hbar}{2}\mathcal{P}} \ . \tag{3.52}$$

One might desire to find state distributions for quantum mechanical systems that mimic the same concept as it appears of classical mechanics: a real-valued, nonnegative function by means of which expectation values of observables can be calculated (a probability distribution). It might be tempting to assume that the sole difference between a classical and a quantum state distribution is that the latter cannot

be too narrow so as to reflect the incomplete knowledge asserted by the Heisenberg uncertainty principle. However, the difference is much more striking.

In the Wigner representation, the state distribution is given by

$$\rho_W = \frac{1}{(2\pi\hbar)^N} \int dq' \, e^{ipq'/\hbar} \left\langle q - \frac{1}{2}q' \right| \hat{\rho} \left| q + \frac{1}{2}q' \right\rangle \ , \tag{3.53}$$

where N is the number of degrees of freedom. The Wigner function has the property that its marginal distributions with respect to p and q give the q and p probability distributions, respectively:

$$\int dp \ \rho_W(q,p) = \langle q|\rho_W|q\rangle = |\psi(q)|^2 \ , \tag{3.54}$$

$$\int dq \ \rho_W(q,p) = \langle p|\rho_W|p\rangle = |\psi(p)|^2 \ . \tag{3.55}$$

However, the Wigner function is not itself a probability distribution. This is due to the fact that the Wigner function takes on negative values in some regions of the phase space [36]. We thus refer to it as a *quasi-probability distribution*.

A class of phase space representations can be obtained from different quantization maps, specifying different operator-ordering recipes. Examples include the standard, anti-standard, normal, anti-normal and Born-Jordan orderings.

Another class can be obtained through a coarse-graining of a given state distribution to produce a new one. An example of this is the generalizaed Husimi distribution which is a special case of a Gaussian smoothing of the Wigner distribution (see [31] and references therein; see also [40]). Note that a Gaussian-smoothed distribution introduces new parameters into a system, the widths of the smoothing Gaussians. Strictly speaking, it is not a representation of quantum mechanics, but a deformation of one, parametrized by the additional variables. We refer to it as a realization.

The Wigner representation and its Gaussian-smoothing are related by

$$\rho_H(q,p) = \int dq'\, dp'\; e^{-\frac{1}{\eta}\left((q-q')^2/s^2 + s^2(p-p')^2\right)} \rho_W(q',p') \;. \tag{3.56}$$

The parameter η controls the area of smoothing in phase space while the parameter s sets the squeezing of this area in q-space and p-space. The Husimi distribution is a Gaussian-smoothed Wigner distribution with smoothing parameter $\eta = \hbar$. It has a $\star$-product

$$\star_H = \mathrm{e}^{\frac{i\hbar}{2}\left[\mathcal{P} - i\sum\left(s^2 \overleftarrow{\partial}_q \overrightarrow{\partial}_q + \overleftarrow{\partial}_p \overrightarrow{\partial}_p/s^2\right)\right]} \;, \tag{3.57}$$

where the sum is implied over all q's and p's. Setting $\eta \geq \hbar$ guarantees that the smoothing size is wide enough to obscure the oscillation of the Wigner function into negative values, rendering the resulting state distribution nonnegative.

The state operator $\hat{\rho}$ is the best candidate to be transformed, via a dequantization map, into a state distribution $\rho = \mathcal{Q}^{-1}(\hat{\rho})$. In the Wigner representation, the expectation value of a dynamical variable f is given by [33]

$$\langle \hat{f} \rangle = \mathrm{Tr}(\hat{\rho}\hat{f}) = \int dq\, dp\; \rho_W \star_W f_W = \int dq\, dp\; \rho_W f_W \;. \tag{3.58}$$

The calculation of expectation values in other realizations is not straightforward. Nonetheless, the general procedure of calculating expectation values of dynamical variables as an integral over phase space is valid. Every *realization* of phase space dynamics comes with both: a $\star$-product and a corresponding map $\hat{f} \to f$.

Finally, we end this section with the equation for the dynamical evolution of the state distribution. Applying the dequantization map to the von Neumann equa-

tion (3.43), we get the quantum analogue of the Liouville equation

$$[\![\rho, H]\!] + \frac{\partial \rho}{\partial t} = 0 \ . \tag{3.59}$$

Note that ρ, H and the $\star$-product giving rise to the bracket $[\![\cdot\,,\cdot]\!]$, all have to be calculated within a particular realization (Wigner, Husimi, etc.).

We have seen in the previous chapter that the classical evolution equation (2.47) descibes an incompressible flow of the state distribution. We can see that the quantum evolution of the state distribution is not incompressible. Expanding the quantum bracket in (3.59) in powers of $\hbar$ we get

$$\{\rho, H\} + \rho \left[\sum_{n=1}^{\infty} \hbar^n \left(\mathcal{G}_{n+1} - \mathcal{G}^t_{n+1} \right) \right] H + \frac{\partial \rho}{\partial t} = 0 \ . \tag{3.60}$$

Then, unless the terms $\rho \left[\sum_{n=1}^{\infty} \hbar^n \left(\mathcal{G}_{n+1} - \mathcal{G}^t_{n+1} \right) \right] H$ vanish, we have

$$\{\rho, H\} + \frac{\partial \rho}{\partial t} \neq 0 \ . \tag{3.61}$$

In general, the $\mathcal{G}_{n>2}$ terms involve higher derivatives that spoil the incompressibility of ρ. This indicates a diffusive evolution of the state distribution.

3.3 The classical limit

Classical mechanics is a successful theory of systems involved in everyday experience or larger. But these systems are ultimately comprised of a large number of small constituents that are quantum mechanical. Thus, if quantum mechanics is to be regarded as a fundamental theory, it must reproduce classical mechanics in some limit.

The classical limit of quantum mechanics is achieved when the physical parameters of the system of interest form a scale S, such that $\hbar/S \to 0$. This has been loosely

stated as simply $\hbar \to 0$. The latter form works intuitively in some cases, like the inequality of the uncertainty principle

$$\Delta q \, \Delta p \geq \frac{\hbar}{2} \;\longrightarrow\; \Delta q \, \Delta p \geq 0 \; . \tag{3.62}$$

In other cases, like the direct application to the Schrödinger equation, it makes little sense. In this respect, the phase space formulation has an advantage over the operator formulation. That is one of the main motivations we adopt it for this work.

We first review three main paths to the classical limit in the operator formulation and point out their shortcomings. This review is largely based on the analysis in [36]. Then we outline how the classical limit is achieved in the phase space formulation and discuss its advantage and some caveats.

3.3.1 The Ehrenfest theorem

The simplest and most famous go-to example of the classical limit is the Ehrenfest theorem. In the Heisenberg picture of the operator formulation, if $\hat{H}$ is the Hamiltonian, then the Heisenberg equations of motion for operators $\hat{q}$ and $\hat{p}$ are

$$\frac{d\hat{q}}{dt} = \frac{1}{i\hbar}[\hat{q}, \hat{H}] \; , \quad \frac{d\hat{p}}{dt} = \frac{1}{i\hbar}[\hat{p}, \hat{H}] \; . \tag{3.63}$$

Here, the commutator $[\hat{A}, \hat{B}]$ is $\hat{A}\hat{B} - \hat{B}\hat{A}$. Taking the expectation value in some state of both sides of these equations, we get

$$\frac{d\langle\hat{q}\rangle}{dt} = \left\langle \frac{1}{i\hbar}[\hat{q}, \hat{H}] \right\rangle \; , \quad \frac{d\langle\hat{p}\rangle}{dt} = \left\langle \frac{1}{i\hbar}[\hat{p}, \hat{H}] \right\rangle \; . \tag{3.64}$$

For simplicity, let us consider the familiar Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \; . \tag{3.65}$$

Then we have

$$\frac{1}{i\hbar}[\hat{q}, \hat{H}] = \hat{p}/m \ , \quad \frac{1}{i\hbar}[\hat{p}, \hat{H}] = F(\hat{q}) \ , \tag{3.66}$$

where $F(\hat{q})$ is the quantum analogue of force. Then, equations (3.64) become

$$\frac{d\langle\hat{q}\rangle}{dt} = \langle\hat{p}\rangle/m \ , \quad \frac{d\langle\hat{p}\rangle}{dt} = \langle F(\hat{q})\rangle \ . \tag{3.67}$$

Now, if $\langle F(\hat{q})\rangle$ can be approximated as

$$\langle F(\hat{q})\rangle \approx F(\langle\hat{q}\rangle) \tag{3.68}$$

then equations (3.67) become

$$\frac{d\langle\hat{q}\rangle}{dt} = \langle\hat{p}\rangle/m \ , \quad \frac{d\langle\hat{p}\rangle}{dt} = F(\langle\hat{q}\rangle) \ . \tag{3.69}$$

The first of these relates $\langle\hat{q}\rangle$ to $\langle\hat{p}\rangle$, the second is Newton's law for them.

The Ehrenfest theorem is the statement that if $\langle F(\hat{q})\rangle \approx F(\langle\hat{q}\rangle)$ is a reasonable approximation, then the expectation values $\langle\hat{q}\rangle$ and $\langle\hat{p}\rangle$ follow a classical evolution.

It might be tempting to interpret the condition $\langle F(\hat{q})\rangle \approx F(\langle\hat{q}\rangle)$ as the classical limit. However, this condition is neither necessary nor sufficient for the classical limit [42]. It is insufficient because this condition is exactly and identically satisfied for any $F(\hat{q})$ that is linear in $\hat{q}$ in *any* state. Quantum systems of free particles and harmonic oscillators have $\langle F(\hat{q})\rangle = F(\langle\hat{q}\rangle)$, yet their behavior is clearly not classical.

Condition (3.68) is not necessary for classical behavior, either. Consider a classical system with a given state distribution so that the classical expectation values $\langle q\rangle$ and $\langle p\rangle$ can be calculated. Then, following the same procedure of taking the expectation

value of Hamilton's equations (2.15) gives

$$\frac{d\langle q\rangle}{dt} = \langle p\rangle / m \ , \quad \frac{d\langle p\rangle}{dt} = \langle F(q)\rangle \ . \tag{3.70}$$

These are evidently identical to their quantum counterparts (3.64). In general, the classical potential and state distribution can be chosen such that $\langle F(q)\rangle \neq F(\langle q\rangle)$. The expectation values, thus, do not follow Newton's law, yet, this *is* a classical system.

We thus see that Ehrenfest's theorem is really about systems described in the framework of Hamiltonian mechanics. The system being classical or quantum is irrelevant. Another indication that Ehrenfest's theorem does not relate to the classical limit is that it involves no $\hbar$'s going to zero anywhere. It defines no scale around which classical behavior arises.

3.3.2 The quantum Hamilton-Jacobi equation

What happens when one takes the limit $\hbar \to 0$ in the central equation of quantum mechanics, the Schrödinger equation?

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi \tag{3.71}$$

As mentioned before, nothing meaningful. However, a simple rewriting of the wave function Ψ, yields a very attractive form of the equation: a direct analogy with the classical Hamilton-Jacobi equation. Indeed, Schrödinger's own "derivation" of his equation was inspired by the optico-mechanical analogy, which is based on the Hamilton-Jacobi equation [43].

Writing the wave function Ψ in terms of its real amplitude R and phase S

$$\Psi(q,t) = R(q,t)e^{-\frac{1}{i\hbar}S(q,t)} \tag{3.72}$$

separates the Schrödinger equation (3.71) into real and imaginary parts

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} = 0 \ , \tag{3.73}$$

$$\frac{\partial R^2}{\partial t} + \nabla \cdot \left(R^2 \frac{\nabla S}{m} \right) = 0 \ . \tag{3.74}$$

The second of these is the continuity equation for the quantum probability distribution in configuration space.

The first equation is the quantum version of the Hamilton-Jacobi equation. The last term in (3.73)

$$V_Q = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} \tag{3.75}$$

is called the *quantum potential*, since it adds to the conventional potential. It is tempting to see a classical limit in equation (3.73). Taking $\hbar \to 0$ gives an equation that is identical to the classical Hamilton-Jacobi equation. However, this is both incorrect and conceptually problematic.

Even though V_Q is formally proportional to $\hbar^2$, one can easily think of wave functions whose amplitudes include factors of $\hbar$. This would spoil the limit $\lim_{\hbar \to 0} V_Q = 0$, giving an equation that is no longer similar to the classical Hamilton-Jacobi equation.

On the other hand, what does "similar" or even "identical" to the classical equation mean? Ψ is the quantum wave function and S is its phase. But in the classical Hamilton-Jacobi equation, S is Hamilton's principal function [44]. An identification between the two quantities is an extra physical assumption, one that is not warranted for cases where $V_Q \neq 0$.

Therefore, despite its attractiveness, the quantum Hamilton-Jacobi equation (3.73) is not a good candidate for a general, consistent calculation of the classical limit.

3.3.3 The large quantum number limit

A common view of the classical limit is one of emergence of classical behavior out of quantum mechanics in states of large quantum numbers. In many quantum systems, like the harmonic oscillator, the position probability distribution $|\Psi|^2$ oscillates in space with shorter wavelengths as the energy goes higher. If the wavelength of the of this oscillation is "small enough", a classical probability distribution can, conceivably, emerge.

The character of this procedure is already familiar. For example, it is the one used in the WKB method [36]. An approximation is made for situations where the oscillation wavelengths is narrow enough that the potential does not change appreciably across this short distance. There is no general treatment for all possible systems.

Obtaining a classical probability distribution involves a *coarse graining* of the highly oscillatory quantum probability distribution. A (length, or otherwise) scale has to be introduced. Such a scale could account for the resolution of the measuring device. It is to this scale that the wavelength is compared, and deemed "small". The higher the quantum number, the shorter the wavelength and the smaller the coarse-graining can be.

We should note that in this account of the classical limit, it is unclear what is meant by "classical behavior". The limit obtained is one of probability distributions. To observers, using measuring devices of finite resolution, quantum probabilities are smeared out according to the state being measured and the minimum resolution. Although "large" systems have probabilities expected from a classical treatment, no reference is made to classical *dynamics* emerging.

3.3.4 Classical limit in phase space

The phase space formulation of quantum mechanics describes quantum dynamical variables in the same language as that of classical mechanics. It captures the

noncommutative nature of the operator formulation by employing the $\star$-product. In section 3.1, we have seen that the quantum dynamical bracket is defined to become the classical Poisson bracket in the limit of $\hbar \to 0$

$$[\![\cdot\,,\cdot]\!] = \{\cdot\,,\cdot\} + \mathcal{O}(\hbar)\ . \tag{3.76}$$

Thus, *the form* of quantum dynamical equations reduces to that of classical ones in the $\hbar \to 0$ limit

$$\left[\frac{d}{dt} = [\![\cdot\,,\cdot]\!] + \frac{\partial}{\partial t}\right] \longrightarrow \left[\frac{d}{dt} = \{\cdot\,,\cdot\} + \frac{\partial}{\partial t}\right]\ . \tag{3.77}$$

Notice that the dynamical variables are missing.

What is described above is the classical limit of *dynamics*. On the other hand, we have the *entities* that flesh out this skeleton: dynamical variables or state distributions. These can contain factors of $\hbar$, which would spoil the straightforward correspondence depicted in (3.77). This is not a bad thing. It draws our attention to the distinction between the *limit of dynamics* and the *limit of entities*.

To illustrate this point, consider a quantum system described by a Hamiltonian that is $\hbar$-free and that is no higher than quadratic in q and p in the Wigner representation. For that system, we identically have

$$[\![\cdot, H]\!] = \{\cdot, H\}\ . \tag{3.78}$$

Time evolution is classical. It is a quantum system, but its state distribution does not diffuse. In fact, for the harmonic oscillator, the Wigner state distribution is nonnegative, just like a classical one [36].

Realizing that the "classical limit" is not a monolithic concept is advantageous for analysis. Phase space quantum mechanics allows us to make that analysis in clear

terms. Quantum systems can have classical evolutions, but classical systems have to be classical all the way: the state distribution must be a probability distribution that is incompressible.

There are several examples of state distributions that, when expanded in powers of $\hbar$, do not reduce the quantum evolution equation to the classical one [26, 45, 46, 39]

$$\frac{d\rho}{dt} = [\![\rho, H]\!] + \frac{\partial \rho}{\partial t} \neq \{\rho_{\hbar\to 0}, H\} + \frac{\partial \rho_{\hbar\to 0}}{\partial t} + \mathcal{O}(\hbar) \ . \tag{3.79}$$

This means that taking the limit of $\hbar \to 0$ is not sufficient to achieve a complete classical limit.

Similar to the discussion in Sec. 3.3.3, a coarse-graining scale needs to be introduced: a minimum resolution for the measuring device that obscures quantum weirdness at short intervals, like negative probabilities in phase space. An example of this the Husimi distribution, which is a Gaussian smoothing of the Wigner distribution (3.56)

$$\rho_H(q,p) = \int dq'\, dp'\ e^{-\frac{1}{\hbar}\left((q-q')^2/s^2 + s^2(p-p')^2\right)}\ \rho_W(q',p') \ . \tag{3.80}$$

The Husimi distribution is real and nonnegative with unit phase space integral, making it a good candidate for a probability distribution [36]. Indeed, using the $\star$-product associated with it, the equation of motion for the Husimi distribution reduces to the Liouville equation in the limit of $\hbar \to 0$ [26].

We see that the phase space formulation is well equipped to give the clearest possible analysis of what constitutes a classical limit.

3.4 Quantum measurement and non-determinism

Perhaps nowhere is the difference between classical and quantum theories more pronounced than in the outcome of measurements. Not only does quantum mechanics

place a fundamental limit on the precision of measurements through the Heisenberg uncertainty principle, it completely changes the rules of the game when a measurement is made. This defining property of quantum mechanics defies satisfactory understanding.

3.4.1 The uncertainty principle

The uncertainty principle states that two noncommuting variables cannot both be measured with perfect precision. This shows that quantum uncertainty is encoded in the noncommutativity of its composition product.

In operator form, the uncertainty relation between operators $\hat{A}$ and $\hat{B}$ is given by

$$\Delta A \, \Delta B \geq \left| \frac{1}{2i} \langle \hat{A}\hat{B} - \hat{B}\hat{A} \rangle \right| \ . \tag{3.81}$$

The uncertainty $\Delta\hat{A}$ is defined as $\sqrt{\left\langle \left(\hat{A} - \langle \hat{A} \rangle \right)^2 \right\rangle}$. Using the fundamental canonical commutation relations (3.27), the famous Heisenberg uncertainty relation for $\hat{q}$ and $\hat{p}$ follow

$$\Delta q \, \Delta p \geq \frac{\hbar}{2} \ . \tag{3.82}$$

The same relation can be obtained from the Wigner representation [47].

It is worth noting, however, that, while $\hbar/2$ is the absolute minimum uncertainty for $\Delta q \, \Delta p$ in any realization, some realizations will have a larger minimum. The Husimi realization, for example, has $\hbar$ as the minimum; twice as large as that of Wigner's [36].

Regardless of the value of the minimum uncertainty, we see that the noncommutativity of the composition product is responsible for the existence of a minimum uncertainty for the simultaneous measurement of canonical conjugates. This noncommutativity then encodes uncertainty into the fundamental laws instead of attributing

it solely to our lack of knowledge as in the classical case. Thus, in quantum mechanics, state distributions are not allowed to be delta functions in phase space. Roughly, in accordance with the uncertainty principle, a quantum state distribution cannot have an area of support smaller than $\hbar/2$.

Even though the the state distribution evolves deterministically (Eq. (3.59)), and so do the observables (Eq. (3.30)), the values of observables are never deterministic. The reason for this is twofold: 1. The state distribution is never a delta function, and 2. The outcome of measurements is intrinsically random.

3.4.2 State collapse: the other law of evolution

Even though the origin of uncertainty is different in quantum and classical mechanics, the subsequent treatment is not much different; there is a state distribution that evolves according to some differential equation. So far, quantum mechanics looks, indeed, like nothing more than a deformation of classical mechanics. But it is more.

When a quantum measurement is made, the smooth, deterministic evolution of the state is interrupted and replaced by an abrupt and random change: a state collapse. This sudden change is incompatible with the dynamical evolution described by the Schrödinger equation [48]. In the language of operator quantum mechanics, dynamical evolution is unitary while the collapse is not.

The incompatibility of the two "modes" of change of quantum systems requires a separate postulate for the act of measurement. This is clearly at odds with reductionism, since the process of measurement should not be any different from an interaction between the quantum system of interest and the measuring device. The measuring device (like the scientist operating it) is made of atoms, and so is a fundamentally quantum mechanical system as well. Two interacting quantum systems should evolve dynamically, so where does the collapse come from? And if all the equations describing interactions are deterministic, where does the randomness fit in?

In classical mechanics, the state distribution is a mere representation of *our* knowledge of the system. We did not have enough information about the system, we made a measurement, and now we know more. Thus, *updating* this knowledge by hand and not by dynamical evolution is perfectly acceptable. But in quantum mechanics, the state distribution is not a probability distribution, it is not simply a description of our knowledge. Plus, the classical lack of knowledge is not fundamental, in contrast to quantum mechanics. An explicit reference to observers, their knowledge and measurements is arguably problematic for a fundamental theory.

The measurement problem is a profound challenge to a complete understanding of quantum mechanics as a fundamental theory. It is beyond the scope of this work to delve more into it (see [5] for a discussion of the problem). Yet, the study of hybrid dynamics in Ch. 4 may shed some light on this problem. The next subsection should provide a reason for this belief.

3.4.3 Copenhagen: classical beings in a quantum world

If the system and the apparatus are both, in the final analysis, quantum, they should evolve into a state of superposition. But we do not see dials pointing up and down at the same time. Is there a mechanism for the collapse of the wave function, or is there a special law of nature for when humans decide to measure things?

There are multiple interpretations of quantum mechanics that try to answer these questions. Conservative attempts try to derive the collapse from the Schrödinger equation of "the environment". Unfortunately, this leads to circular arguments. On the other hand, adventurous proposals deny the collapse ever happens, but they come at a heavy cost. Others modify quantum mechanics by adding hidden variables or nonlinearity. Yet others assert that physics is fundamentally about humans trying to describe the universe, quantum mechanics is about our knowledge and not what is "really" out there. The fact that there is no consensus among physicists on the

interpretation of quantum mechanics tells us something about the success of these solutions.

These revolutionary ideas find their common origin in the (legitimate) dissatisfaction with the original picture of quantum mechanics, if there ever was one picture of it. The orthodox Copenhagen understanding of quantum mechanics is, understandably, confusing.

The orthodox view is that, in a quantum measurement, the measuring apparatus must be treated classically. In the words of Landau and Lifshitz, *"[Q]uantum mechanics occupies a very unusual place among physical theories: it contains classical mechanics as a limiting case, yet at the same time it requires this limiting case for its own formulation."* [49]. The use of this limiting case to account for the process of measurement was never shown, which led to the aforementioned attempts and many others.

A consistent framework for studying the interaction between quantum and classical systems might help study the measurement problem in the orthodox spirit. While it will inherit the ambiguity of defining where lies this limit, it would be a step towards providing a mechanism for measurement in terms of familiar interaction.

Chapter 4

Hybrid Quantum-Classical Dynamics

We have seen that quantum and classical theories share the same formal structure of Hamiltonian dynamics. Minimum uncertainties, nonlocalities and negative probabilities notwithstanding, both frameworks transform variables using dynamical brackets and use state distributions to specify expectation values. As a reminder, we emphasize that a dynamical bracket is a Lie bracket that obeys the Leibniz rule with respect to an associative composition product. The measurement problem aside, the algebra of quantum observables is nothing more than a deformation of that of classical observables: unusual and interesting, but formally similar.

In this chapter, we leverage their similarity to investigate the combination of quantum and classical mechanics into a single framework. We would like that framework to have the same formal Hamiltonian structure.

Several proposals for hybrid quantum-classical dynamics can be found in this incomplete list [11, 12, 50, 51, 52]. See also [53, 54, 55, 56] and the references therein. On the other hand, no-go theorems in [14, 15, 16, 17, 18] argue that no hybrid bracket can describe consistent dynamics, on account of the bracket violating the Jacobi identity and the Leibniz rule. The goal of this work is to study the construction of a framework that generalizes previous attempts, and explore possible ways of keeping such framework consistent. The results presented here are based on our work in [20].

4.1 What's it good for?

If classical mechanics is but a limiting case of quantum mechanics, of what use is their hybridization? Would that just be an approximation? An approximation can lead to nonsensical results if pushed outside its domain of validity. On the other hand, a consistent, autonomous approximation can illuminate the character of the approximated. For example, nonrelativistic mechanics is an approximation of relativistic mechanics, but it is a self-consistent one that stands on its own, which is then used as a template for building its (logically) parent theory. We can learn which aspects of a given quantum theory can be captured classically, and which ones are irreducibly quantum.

As an example, consider the problem of quantum gravity. No quantum theory of gravity enjoys the consensus of physicists, yet all attempts at this elusive theory learn from the study of quantum field theory on a classical curved background. This is an example of a hybrid system, albeit an incomplete one; it does not consider the effect of the quantum fields on the gravitational field. If a consistent treatment of the interaction (action of the classical on the quantum and back-reaction of the quantum on the classical) exists, then that would be an autonomous first approximation that might serve as a guide to the construction of a quantum theory of gravity. Such a framework would also be more directly beneficial for studying quantum fluctuations in the early universe or the behavior of matter near a black hole singularity.

For a more applied example, consider calculations/simulations of fully quantum systems. Performing these calculations for systems of many degrees of freedom is computationally expensive. It would be more feasible if some degrees of freedom could be treated classically while still receiving influence from the quantum degrees of freedom. The effect of quantum electrons on "classical" nuclei is an interesting instance [3].

Motivation for studying quantum-classical interaction can also be found on the

foundational front. We quote Landau and Lifshitz again *"[Q]uantum mechanics occupies a very unusual place among physical theories: it contains classical mechanics as a limiting case, yet at the same time it requires this limiting case for its own formulation."* [49]. A detailed, consistent treatment of the act of measurement as a quantum-classical interaction in a hybrid system might provide a mechanism for the state collapse. This could shed new light on the orthodox interpretation of quantum mechanics.

And finally, we return one more time to gravity. What if gravity is fundamentally classical? This possibility was argued against in the past based on the inconsistency of combining classical and quantum mechanics (see [19] and the references therein). What if this inconsistency can be re-examined, and that hybrid dynamics is a possible option? That certainly is an interesting path to explore.

4.2 A general quantum-classical bracket

In this section, we derive a generalized form of the hybrid quantum-classical dynamical bracket. We start with the assumption that quantum dynamics is fundamental, so that classical dynamics arises as a limit of it, as discussed in Sec. 3.3. We then divide the full quantum system into Q- and C-sectors and take the classical limit only for the C-sector degrees of freedom. In that procedure, we use the phase space formulation.

The result of the partial application of the classical limit produces a C-sector that has no memory of ever being quantum, at least as far as dynamics is concerned (we are not discussing state distributions). Indeed, we also show that if classical dynamics is treated on an equal footing with quantum dynamics, the same formal bracket can be constructed without recourse to a partial classical limit.

4.2.1 Basic requirements

In constructing a hybrid bracket, some natural requirements can serve as guidance. There is the general requirement of being a Lie bracket that obeys the Leibniz rule with respect to a suitable composition product. Besides that, we impose the more specific *reduction requirement*: the hybrid bracket should reduce to a pure quantum or classical bracket if one of its arguments is pure of the same type (see [15])

$$\{[\text{Quantum}\,,\text{Hybrid}]\} = [\![\text{Quantum}\,,\text{Hybrid}]\!]\ , \tag{4.1a}$$

$$\{[\text{Classical}\,,\text{Hybrid}]\} = \{\text{Classical}\,,\text{Hybrid}\}\ . \tag{4.1b}$$

Here, $\{[\cdot\,,\cdot]\}$ represents a hybrid bracket. This requirement is natural if we consider pure variables to be a special case of hybrid variables. Note that all three brackets vanish when one argument is quantum and the other is classical, since these variables belong to different sectors and are independent degrees of freedom.

The first of equations (4.1) describes a situation that is already familiar: textbook quantum mechanics. Consider a quantum particle with Hamiltonian $H = p^2/2m + V(q)$. The potential $V(q)$ represents the action of some external influence on the quantum particle. The source of this external influence is not affected by the quantum particle. This is good enough for all practical purposes. But from a fundamental point of view, it is unphysical to have an external effect devoid of dynamics. The fact that we consider the source of the external potential to be completely stationary is a testament to the assumption that it is classical [1]. Quantum sources cannot have a well defined position and momentum and thus cannot define a rigid, stationary potential.

A more realistic Hamiltonian for textbook quantum mechanics would be

$$H = \frac{p_Q^2}{2m_Q} + \frac{p_C^2}{2m_C} + H_I(q_Q, q_C)\ . \tag{4.2}$$

The subscripts Q and C refer to quantum and classical respectively and H_I refers to

the interaction between them. The basic assumption is that the effect of the quantum particle on the classical source of the potential can be ignored. Thus, the potential is stationary, i.e., $p_C = 0$, thus making q_C constant. Then we end up with

$$H = \frac{p_Q^2}{2m_Q} + H_I(q_Q, q_C = \text{const.}) = \frac{p_Q^2}{2m_Q} + V(q_Q) \ . \tag{4.3}$$

We see that textbook quantum mechanics (and similarly, in a formal sense, QFT on a curved background) is a special case of hybrid dynamics. And since that familiar situation is described in terms of the quantum dynamical bracket, and not the hybrid one, we must have

$$\{[\text{Quantum}\,,\text{Hybrid}]\} = [\![\text{Quantum}\,,\text{Hybrid}]\!] \ . \tag{4.4}$$

The action of the classical on the quantum is built-in in quantum mechanics. It is the reverse effect, the back-reaction, that is elusive. Nonetheless, we assume the symmetry of treatment of pure quantum and classical variables to motivate the second of equations (4.1).

4.2.2 The partial classical limit

Let a set of degrees of freedom and their conjugate momenta be subdivided into two sectors (1) and (2). We refer the canonical conjugates belonging to sector (1), collectively, as (q_1, p_1), and similarly for sector (2). Any variable in the full system can be represented as

$$u(q_1, p_1, q_2, p_2) = \sum u_1(q_1, p_1)\, u_2(q_2, p_2) \ . \tag{4.5}$$

Without loss of generality, we will only consider only a single term of this sum from now on ($u = u_1\, u_2$). Notice that, since u_1 and u_2 are independent, they commute.

The $\star$-product acting on the full system can be factorized as

$$\star_{\text{Full}} = \star_1 \star_2 = \star_2 \star_1 \ . \tag{4.6}$$

The two product operators commute since they operate on independent systems so that we have

$$u \star_{\text{Full}} v = (u_1 \star_1 v_1)\,(u_2 \star_2 v_2) \ . \tag{4.7}$$

This is clear from the operator representation

$$(\hat{A}_1 \hat{A}_2)\,(\hat{B}_1 \hat{B}_2) = (\hat{A}_1 \hat{B}_1)\,(\hat{A}_2 \hat{B}_2) \ . \tag{4.8}$$

Note that the two systems may, and will, interact. They are independent in the sense that the canonical coordinates are geometrically independent (no constraints). This ensures that commutators of variables belonging to different sectors vanish.

Since the two subsystems are independent, $\star_1$ and $\star_2$ are not restricted to be of the same realization. It is possible to have Wigner on one sector and Husimi on the other, for example.

With the system subdivided into Q- and C-sectors, we now expand the $\star_C$-product alone

$$\star_{\text{Full}} = \star_Q \star_C = \star_Q \left(1 + i\hbar_C\, \mathcal{G}_{1C} + \mathcal{O}(\hbar_C^2)\right) \ . \tag{4.9}$$

The full dynamical bracket is then expanded as

$$[\![\cdot\,,\cdot]\!]_{\text{Full}} = \frac{1}{i\hbar}\left(\star_{\text{Full}} - \star^t_{\text{Full}}\right) \tag{4.10}$$

$$= [\![\cdot\,,\cdot]\!]_Q + \frac{\hbar_C}{\hbar}\left(\star_Q \mathcal{G}_{1C} - \star^t_Q \mathcal{G}^t_{1C}\right) + \mathcal{O}\left(\hbar_C^2/\hbar\right) \ . \tag{4.11}$$

Where $\hbar_C$ is Planck's constant on the classical sector.

Of course, Planck's constant is *constant*, but we leave the subscript C as a book-keeping device. The dynamical bracket $[\![\cdot\,,\cdot]\!]_Q$ on the quantum sector contains powers of $\hbar$ as well, yet only terms of order $\hbar_C^2/\hbar$ will be approximated to zero. The term $\mathcal{O}(\hbar_C^2/\hbar)$ is taken to be vanishingly small compared to a scale of action on the classical sector

$$\sum_{n=2}^{\infty} \frac{\hbar_C^n}{\hbar} \Big[(u_Q \star_Q v_Q)\,(u_C\,\mathcal{G}_{nC}\,v_C) - (v_Q \star_Q u_Q)\,(v_C\,\mathcal{G}_{nC}\,u_C) \Big] = \mathcal{O}(\hbar_C^2/\hbar)\ . \tag{4.12}$$

We see that this scale will be defined by the terms $u_C\,\mathcal{G}_{nC}\,v_C$. After the limit is taken, $\hbar_C$ can be set to equal $\hbar$ at will.

Taking the limit $\hbar_C^2/\hbar \to 0$, we arrive at the hybrid bracket

$$\{[\cdot\,,\cdot]\} := [\![\cdot\,,\cdot]\!] + \frac{\hbar_C}{\hbar}(\star\mathcal{G} - \star^t\mathcal{G}^t)\ . \tag{4.13}$$

From now on, the subscripts on $\star$ and $\mathcal{G}$ as well as pure quantum or pure classical brackets will be dropped. It should be understood that $\star$ and $[\![\cdot\,,\cdot]\!]$ act only on Q-variables while $\mathcal{G} := \mathcal{G}_{1C}$ and $\{\cdot\,,\cdot\}$ act only on C-variables.

Since the Poisson bracket $\mathcal{P}$ is the commutator of the $\mathcal{G}$-product, we can write $\mathcal{G}$ in terms of its symmetric and antisymmetric parts

$$\mathcal{G} = \frac{1}{2}(\mathcal{P} + \sigma)\ , \tag{4.14}$$

where σ is a symmetric product. Note that the antisymmetric part is fixed to be the Poisson bracket, while the symmetric part has some freedom since σ is, thus far, unconstrained. The hybrid bracket can then be rewritten as

$$\{[\cdot\,,\cdot]\} = [\![\cdot\,,\cdot]\!] + \frac{\hbar_C}{\hbar}\left(\frac{\star+\star^t}{2}\mathcal{P} + \frac{\star-\star^t}{2}\sigma\right)\ . \tag{4.15}$$

If we define a classical product

$$\circledast := 1 + i\hbar_C \mathcal{G} = 1 + \frac{i\hbar_C}{2}(\mathcal{P} + \sigma) \ , \tag{4.16}$$

then the hybrid bracket takes a more symmetric form:

$$\{\![\cdot\,,\cdot]\!\} = \frac{1}{i\hbar}[\star\circledast - \star^t\circledast^t] \ . \tag{4.17}$$

This form will be instrumental in studying the properties, and consistency conditions for the hybrid bracket. Note that $\circledast$ is a semiclassical approximation of $\star_C$, and since $\mathcal{G} - \mathcal{G}^t = \mathcal{P}$, we have

$$\{\cdot\,,\cdot\} = \frac{1}{i\hbar_C}[\circledast - \circledast^t] \ . \tag{4.18}$$

The hybrid bracket is automatically antisymmetric and linear. The requirement that it to obeys the Jacobi identity and Leibniz rule will be discussed in detail in Sec. 4.4. The bracket as it is, however, does possess a *quasi-Leibniz* property. Consider two hybrid variables u and $v = v_Q v_C$. From (4.13) and (4.16) we can show that

$$\{\![u, v]\!\} = [\![u, v_Q]\!] \circledast v_C + v_Q \star \{u, v_C\} \tag{4.19}$$

$$= \{\![u, v_Q]\!\} \circledast v_C + v_Q \star \{\![u, v_C]\!\} \ . \tag{4.20}$$

This shows that if both pure variables v_Q and v_C commute with u, then so does $(v_Q v_C)$, with obvious implications for symmetry.

4.2.3 An alternative route

As mentioned before, the resulting hybrid bracket has no memory of the quantum origin of its classical part. Here, we show that the bracket will have the same form as (4.13) using only the reduction equations (4.1).

Consider a quantum (Q-) system and a classical (C-) system whose canonical coordinates are independent from each other. Since the two systems are independent, then an antisymmetric bracket can be built as

$$\{\![\cdot\,,\cdot]\!\} = \frac{1}{a}[\star\diamond - \star^t\diamond^t]\ , \tag{4.21}$$

where a is an undetermined constant, $\star$ is the familiar quantum product and $\diamond$ is a noncommutative product acting on the classical variables.

From the first of the reduction conditions (4.1) we get

$$\{\![u, v_Q]\!\} = [\![u, v_Q]\!] \tag{4.22}$$

$$\frac{1}{a}\left[(u_Q \star v_Q)\,(u_C \diamond 1) - (v_Q \star u_Q)\,(1 \diamond u_C)\right] = \frac{1}{i\hbar}(u_Q \star v_Q - v_Q \star u_Q)u_C\ . \tag{4.23}$$

By inspection, we see that for this equality to hold, we must have

$$u_C \diamond 1 = 1 \diamond u_C = \frac{a}{i\hbar}u_C\ . \tag{4.24}$$

From the second of (4.1), we have

$$\{\![u, v_C]\!\} = \{u, v_C\} \tag{4.25}$$

$$\frac{1}{a}\,(u_C \diamond v_C - v_C \diamond u_C) = \{u_C, v_C\}\ . \tag{4.26}$$

We can split $\diamond$ into two parts:

$$\diamond = a\left(\frac{1}{i\hbar} + g\right)\ . \tag{4.27}$$

This satisfies both (4.24) and (4.26) if

$$g - g^t = \{\cdot\,,\cdot\} \quad \text{and} \quad 1\,g\,\cdot = 0\ . \tag{4.28}$$

We can see immediately that choosing the constant $a = \hbar$ and the product $g = \mathcal{G}$ yields an expression for $\diamond$ identical to $\circledast$ in (4.16) with $\hbar_C = \hbar$.

The form of the hybrid bracket is more general than its derivation through the partial classical limit of a quantum bracket. This corroborates the assertion that the classical part of the hybrid bracket loses memory of its quantum origin, if it had any.

In obtaining the classical limit in the previous subsection, we argued for the existence of a scale of action on the classical side that is much larger than $\hbar$, warranting the approximation. Here we offer a different argument: we carry out the approximation because we want to. If we consider the logical possibility that quantum-classical mechanics is fundamental, then we *define* some degrees of freedom to be classical and study the problem in that regime. Finding the domain of approximation is besides the point.

4.2.4 The bracket in operator form

The phase space formulation was used to derive the hybrid bracket. This does not prevent us from expressing the bracket in terms of operators. Since operators are most familiar to some, the alternative expression may be helpful.

Define operator $\hat{A}$ as

$$\hat{A} = \hat{A}_Q(q_Q, p_Q) \cdot A_C(q_C, p_C) \ . \tag{4.29}$$

Where, as usual, subscripts indicate the sector to which a variable belongs. Eq. (4.15) can be rewritten as

$$\{\![\hat{A}, \hat{B}]\!\} = \frac{1}{i\hbar}[\hat{A}, \hat{B}] + \frac{1}{2}\frac{\hbar_C}{\hbar}\left(\{\hat{A}, \hat{B}\} - \{\hat{B}, \hat{A}\} + \hat{A}\sigma\hat{B} - \hat{B}\sigma\hat{A}\right) \ . \tag{4.30}$$

The quantum commutator is $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

In terms of the $\circledast$ semiclassical product, the bracket in operator form becomes

$$\{[\hat{A},\hat{B}]\} = \frac{1}{i\hbar}\left(\hat{A}\circledast\hat{B} - \hat{B}\circledast\hat{A}\right) \ . \tag{4.31}$$

The operator form of the hybrid bracket suggests the extension of its validity to act on spin operators as well as canonical ones.

4.2.5 The special case of Wigner

If we consider the quantum origin of the classical sector, then $\mathcal{G}$ (and, by extension, σ) is determined by the choice of quantization (deformation) on the C-sector prior to taking the partial classical limit. In the case of choosing the Wigner realization on the C-sector, we have

$$\circledast = \lim_{\hbar_C^2\to 0} e^{\frac{i\hbar_C}{2}\mathcal{P}} \ , \tag{4.32}$$

so $\sigma = 0$. The hybrid bracket in this case is

$$\{[\cdot\,,\cdot]\} = [\![\cdot\,,\cdot]\!] + \frac{\hbar_C}{\hbar}\frac{\star+\star^t}{2}\mathcal{P} \ . \tag{4.33}$$

In operator form, setting $\hbar_C = \hbar$, the bracket obtained from the Wigner representation is

$$\{[\hat{A},\hat{B}]\} = \frac{1}{i\hbar}[\hat{A},\hat{B}] + \frac{1}{2}\left(\{\hat{A},\hat{B}\} - \{\hat{B},\hat{A}\}\right) \ . \tag{4.34}$$

This form has been proposed in [11] and derived from a partial Wigner transform in [15]. Here, it is a special case of the general hybrid bracket (4.30) with $\sigma = 0$. The Wigner phase space realization is not the only one producing bracket (4.34), the realization based on the Born-Jordan ordering, also, has a vanishing σ.

This bracket has been criticized in [15] for failing to satisfy the Jacobi identity or

the Leibniz rule. We shall address these issues in Sec. 4.4.

4.3 Properties of the general hybrid bracket

The general quantum-classical bracket presented thus far satisfies only two of our requirements: antisymmetry and linearity. The other requirements are that the bracket obeys the Jacobi identity and the Leibniz rule, and that it reduces to pure brackets for pure variables as in equations (4.1). Before tackling the Jacobi and Leibniz conditions in general terms, we can explore what the bracket has to offer considering only the reduction conditions (4.1).

For convenience, we repeat the reduction conditions here

$$\{\![u_Q\,,v]\!\} = [\![u_Q\,,v]\!]\ , \tag{4.35a}$$

$$\{\![u_C\,,v]\!\} = \{u_C\,,v\}\ , \tag{4.35b}$$

where u_Q and u_C are pure quantum and classical variables, respectively, and v is a hybrid variable. We see that as long as one argument of the bracket is pure, then the bracket is pure, and so it becomes automatically consistent (Jacobi- and Leibniz-compliant), since pure brackets are consistent.

This seemingly trivial observation hides interesting details. One of the main motivations of studying hybrid dynamics is to account for the quantum back-reaction *on the classical sector*. The reduction conditions are enough to reveal some aspects of this. Back-reaction is described by a bracket where one argument is the classical variable to be acted upon, and the other argument is an interaction term in the Hamiltonian of the full system.

Since the hybrid bracket becomes pure when one of its arguments is pure, then we

can define time evolution as

$$\frac{du_{\text{Pure}}}{dt} = \{\![u_{\text{Pure}}, H]\!\} + \frac{\partial u_{\text{Pure}}}{\partial t} \ . \tag{4.36}$$

We were able to define this equation because $\{\![u_{\text{Pure}}, \cdot]\!\}$ is a conistent bracket (Leibniz-compliant, in particular). Furthermore, if we admit only one hybrid variable into the theory to serve as an interaction term in the Hamiltonian, then time evolution for any function of that variable can also be defined. This will be useful in the discussion of back-reaction in Sec. 4.3.4.

4.3.1 Reduction to pure quantum mechanics

Using the form of the hybrid bracket (4.15),

$$\{\![u_Q, v]\!\} = [\![u_Q, v_Q]\!]v_C + \frac{\hbar_C}{\hbar}\left(u_Q \frac{\star + \star^t}{2} v_Q \ \{1, v_C\} + u_Q \frac{\star - \star^t}{2} v_Q \ 1 \,\sigma\, v_Q\right) \tag{4.37}$$

$$= [\![u_Q, v]\!] + [\![u_Q, v_Q]\!] \ \frac{i\hbar_C}{2}(1 \,\sigma\, v_C) \ , \tag{4.38}$$

for $v = v_Q v_C$. We see that for the desired reduction ($\{\![u_Q, \cdot]\!\} = [\![u_Q, \cdot]\!]$), we must impose the condition

$$1 \,\sigma\, \cdot = 0 \ ; \tag{4.39}$$

the σ-product annihilates constants. Since $\mathcal{G} = (\mathcal{P} + \sigma)/2$, then $\mathcal{G}$, also, annihilates constants. This is not surprising. Condition (4.39) is satisfied by known phase space realizations since for them, $\mathcal{G}$ is a bidifferential operator.

4.3.2 Action of the classical on the quantum

As discussed in Sec. 4.2.1, textbook quantum mechanics arises from the reduction condition. We repeat the result here for the slightly more interesting case of a

dynamical external classical potential.

For the Hamiltonian $H = H_Q + H_C + H_I$, the evolution of any quantum variable u_Q is given by

$$\frac{du_Q}{dt} = [\![u_Q, H_Q]\!] + [\![u_Q, H_I]\!] + \frac{\partial u_Q}{\partial t} \ . \tag{4.40}$$

The term H_I can be viewed as a time-dependent potential as far as the Q-sector is concerned:

$$H_I\big(q_Q, p_Q, q_C(t), p_C(t)\big) = V(q_Q, p_Q, t) \ . \tag{4.41}$$

If the quantum influence on q_C and p_C is ignored, we get a description of a quantum system on a dynamical classical background.

4.3.3 Reduction to pure classical mechanics

From Eq. (4.15), we have

$$\{\![u_C, v]\!\} = [\![1, v_Q]\!] v_C + \frac{\hbar_C}{\hbar}\left(1\frac{\star + \star^t}{2} v_Q \ \{u_C, v_C\} + 1\frac{\star - \star^t}{2} v_Q \ u_C \, \sigma \, v_Q\right) \tag{4.42}$$

$$= \frac{\hbar_C}{\hbar}\{u_C, v\} \ . \tag{4.43}$$

The hybrid bracket reduces to the classical Poisson bracket rescaled by $\hbar_C/\hbar$. As discussed in Sec. 4.2.2, the subscript C in $\hbar_C$ is left as a device for keeping track of which quantities are to vanish in the classical limit. In the above expression, there is no need to differentiate between $\hbar_C$ and $\hbar$, and we can simply set $\hbar_C/\hbar = 1$. Yet, we still keep the distinction to allow for the possibility of Planck's constant being different in different sectors. The nonuniqueness of Planck's constant was studied in [16, 18] and used to argue for the inconsistency of hybrid dynamics. In our analysis, this point is irrelevant.

If we entertain the notion that $\hbar_C/\hbar \neq 1$, the reduction of the hybrid bracket to a rescaled Poisson bracket is not worrisome. It is a constant, global rescaling that does not alter the dynamics. If $\{\cdot\,,\cdot\}$ is an admissible classical dynamical bracket (a Lie bracket that obeys the Leibniz rule with respect to point-wise multiplication), then so is $\{\cdot\,,\cdot\}' = c\,\{\cdot\,,\cdot\}$, where c is an arbitrary constant. If we do not set $\hbar_C = \hbar$ (and we have no reason not to), then this will have the effect of rescaling all time derivatives. For example, for $H = p_C^2/2m + V(q_C)$ and $F = -V'(q_C)$, we get

$$\dot{q}_C = \{\![q_C, H]\!\} = \frac{\hbar_C}{\hbar}\,\frac{p_C}{m}, \quad \dot{p}_C = \{\![p_C, H]\!\} = -\frac{\hbar_C}{\hbar}\,V'(q_C) \tag{4.44}$$

$$\Rightarrow \quad \left(\frac{\hbar_C}{\hbar}\right)^2 F = m\,\ddot{q}_C\ . \tag{4.45}$$

4.3.4 Quantum back-reaction

Similar to the case of pure quantum variables, pure classical variables that evolve according to the Hamiltonian $H = H_Q + H_C + H_I$ obey

$$\frac{du_C}{dt} = \{u_C, H_C\} + \frac{\hbar_C}{\hbar}\{u_C, H_I\} + \frac{\partial u_C}{\partial t}\ . \tag{4.46}$$

The term $\{u_C, H_I\}$ is the back-reaction contribution to the evolution of u_C.

Like the discussion of the action of classical variables on quantum ones in Sec. 4.3.2, the interaction Hamiltonian H_I can be viewed as

$$H_I(q_Q, p_Q, q_C, p_C) = H_I\big(q_Q(t), p_Q(t), q_C, p_C\big) = H_I(t, q_C, p_C)\ . \tag{4.47}$$

From the C-sector point of view, the quantum back-reaction is expressed in the non-classical explicit time-dependence of H_I. This explicit time dependence is due to the quantum evolution of q_Q and p_Q in H_I.

Let us now consider how H_I evolves in time. Let $\eta(q_Q, p_Q, q_C, p_C)$ be some hybrid

variable that defines the interaction H_I as

$$H_I(q_Q, p_Q, q_C, p_C) = H_I\big(\eta(q_Q, p_Q, q_C, p_C)\big) \ . \tag{4.48}$$

Now, the hybrid bracket of any function of η with the Hamiltonian is

$$\{\![f(\eta), H]\!\} = [\![f(\eta), H_Q]\!] + \frac{\hbar_C}{\hbar}\{f(\eta), H_C\} \ . \tag{4.49}$$

Further, the bracket of any $\star$-composed functions of η with the Hamiltonian obeys the Leibniz rule with respect to the $\star$-product:

$$\begin{aligned} \{\![f(\eta) \star g(\eta), H]\!\} &= [\![f(\eta), H_Q]\!] \star g(\eta) + f(\eta) \star [\![g(\eta), H_Q]\!] \\ &\quad + \frac{\hbar_C}{\hbar}\{f(\eta), H_C\} \star g(\eta) + \frac{\hbar_C}{\hbar} f(\eta) \star \{g(\eta), H_C\} \end{aligned} \tag{4.50}$$

$$= \{\![f(\eta), H]\!\} \star g(\eta) + f(\eta) \star \{\![g(\eta), H]\!\} \ . \tag{4.51}$$

Notice that $\star$ is the composition product that comes to mind for hybrid variables since $u \star v = (u_Q \star v_Q)\,(u_C v_C)$; each pure factor is composed with its familiar composition product. We will see in Sec. 4.4 that a more complicated composition product will allow consideration of a more general case.

This Leibniz property means that $\{\![\cdot\,, H]\!\}$ acts as a derivative for all functions of η. Thus, we can define time evolution of any function $f(\eta)$ in terms of its hybrid bracket with H:

$$\frac{df(\eta)}{dt} = \{\![f(\eta), H]\!\} + \frac{\partial f(\eta)}{\partial t} \tag{4.52}$$

$$= [\![f(\eta), H_Q]\!] + \frac{\hbar_C}{\hbar}\{f(\eta), H_C\} + \frac{\partial f(\eta)}{\partial t} \ . \tag{4.53}$$

Then the interaction term $H_I(\eta)$ evolves as

$$\frac{dH_I}{dt} = [\![H_I, H_Q]\!] + \frac{\hbar_C}{\hbar}\{H_I, H_C\} + \frac{\partial H_I}{\partial t} \ . \tag{4.54}$$

We see that the back-reaction term $\{u, H_I\}$ in (4.46) is controlled by a variable (H_I) that has a hybrid evolution.

4.4 Consistency of hybrid dynamics

Now we turn to the general treatment of quantum-classical mechanics with hybrid variables. Multiple no-go theorems have shown that the bracket (4.34), originally proposed in [11, 12], violates the Jacobi identity and the Leibniz rule [14, 15, 16, 17, 18].

We derive a precise mathematical condition for consistency. This allows us to cast the problem in more manageable terms. As a consequence, we are able to show how, in principle, the no-go theorems may be circumvented.

The general hybrid bracket derived in Sec. 4.2 is identically antisymmetric and linear. However, it does not obey the Jacobi identity in general. But before considering whether or not the bracket obeys the Leibniz rule, we should ask "with respect to which product?". What could serve as a *composition product* for hybrid variables? In this section we attempt to answer these questions and provide a single condition that guarantees the Jacobi and Leibniz conditions and provides a suitable composition product for the latter.

4.4.1 The Jacobi relation

Using the form (4.17), we see that, apart from a factor of $1/i\hbar$, the bracket is a commutator of the $(\star\circledast)$-product. Thus if $(\star\circledast)$ is associative, then the bracket will obey the Jacobi identity.

To see this explicitly, we expand the Jacobi expression for hybrid variables $u =$

$u_Q u_C$, $v = v_Q v_C$ and $w = w_Q w_C$:

$$\begin{aligned}
&\{[\{[u,v]\},w]\} + \{[\{[v,w]\},u]\} + \{[\{[w,u]\},v]\} \\
&\quad = (u_Q \star v_Q \star w_Q)\,[u_C, v_C, w_C]_\circledast \; + \\
&\quad + (v_Q \star w_Q \star u_Q)\,[v_C, w_C, u_C]_\circledast \; + \\
&\quad + (w_Q \star u_Q \star v_Q)\,[w_C, u_C, v_C]_\circledast \; + \\
&\quad + \;\text{ anticyclic permutations of } (u, v, w)\ .
\end{aligned} \tag{4.55}$$

Here, the *associator* with respect to the $\circledast$-product is defined as

$$[u_C, v_C, w_C]_\circledast := (u_C \circledast v_C) \circledast w_C - u_C \circledast (v_C \circledast w_C)\ . \tag{4.56}$$

If the associator $[\cdot\,,\cdot\,,\cdot]_\circledast$ vanishes, the Jacobi identity is satisfied.

The $\circledast$-product is defined as $1 + i\hbar_C \mathcal{G}$. As shown in Sec. 3.1.1, if $\mathcal{G}$ is considered as the first-order term in the expansion of the full quantum $\star_C$-product, then the associativity of $\star_C$ implies that

$$(u_C\, v_C)\, \mathcal{G}\, w_C + (u_C\, \mathcal{G}\, v_C)\, w_C = u_C\, (v_C\, \mathcal{G}\, w_C) + u_C\, \mathcal{G}\, (v_C\, w_C)\ . \tag{4.57}$$

This is a repetition of Eq. (3.11). Using this relation, the $\circledast$-associator can be shown to be equal to the $\mathcal{G}$-associator:

$$[\cdot\,,\cdot\,,\cdot]_\circledast = [\cdot\,,\cdot\,,\cdot]_\mathcal{G}\ . \tag{4.58}$$

The Jacobi identity then requires the associativity of the $\mathcal{G}$-product.

4.4.2 The Leibniz rule

The associativity of the $\circledast$-product demanded by the Jacobi identity immediately provides a suitable composition product for the Leibniz rule. As an identity, the

commutator of an associative product obeys the Leibniz rule with respect to that product:

$$\{\![u \star\circledast v, w]\!\} = \{\![u, w]\!\} \star\circledast v + u \star\circledast \{\![v, w]\!\} \ . \tag{4.59}$$

Thus this single condition, $[\cdot\,,\cdot\,,\cdot]_{\circledast} = 0$, guarantees the consistency of the quantum-classical bracket.

From this result, we realize that $(\star\circledast)$ acts as a natural composition product for hybrid variables. In [16, 18], it was argued that the bracket (4.34)

$$\{\![\hat{A}, \hat{B}]\!\} = \frac{1}{i\hbar}[\hat{A}, \hat{B}] + \frac{1}{2}\Big(\{\hat{A}, \hat{B}\} - \{\hat{B}, \hat{A}\}\Big) \tag{4.60}$$

does not satisfy the Leibniz rule for general hybrid variables. But it was the Leibniz rule with respect to $\star$, not $(\star\circledast)$ that was studied. In operator form, [16, 18] found that

$$\{\![\hat{A}\hat{B}, \hat{C}]\!\} \neq \{\![\hat{A}, \hat{C}]\!\}\hat{B} + \hat{A}\{\![\hat{B}, \hat{C}]\!\} \ , \tag{4.61}$$

which, in phase space form, becomes

$$\{\![u \star v, w]\!\} \neq \{\![u, w]\!\} \star v + u \star \{\![v, w]\!\} \ . \tag{4.62}$$

We see that the result of the no-go theorem in [16, 18] applies for the special case where $\circledast = 1$.

This is where the innovation of $\circledast = 1 + i\hbar_C \mathcal{G}$ is most visible. Realizing the concept of nontrivial composition products inspires exploring the possibility of circumventing these no-go theorems as shown in the rest of this chapter.

4.4.3 Composition product(s) for hybrid dynamics

The fact that the quantum-classical bracket obeys the Leibniz rule with respect to the $(\star\circledast)$-product suggests its role as a composition product for hybrid variables. This, of course, is true only when $\circledast$ is associative since $\star$ already is. This, however, is not the composition product for hybrid variables that is expected at first glance.

If $\star_C$ is the full quantum composition product for the C-sector, expanding it in powers of $\hbar_C$ gives

$$\star_C = 1 + i\hbar_C \mathcal{G} + \mathcal{O}(\hbar_C^2) \ . \tag{4.63}$$

We recover the classical composition product in the limit $\hbar_C \to 0$. So, one would expect that the hybrid composition product would be obtained the same way from the full quantum product (4.7)

$$\star_{\text{Full}} = \star \left(1 + \mathcal{O}(\hbar_C)\right) \longrightarrow \star 1 = \star \ . \tag{4.64}$$

But, as discussed in the previous subsection, $\star$ cannot serve as a composition product for hybrid variables since the Leibniz rule would not be satisfied with respect to it.

On the other hand, the $\circledast$-product is a semiclassical approximation obtained from $\star_C$ in the limit of $\hbar_C^2 \to 0$. Thus, *hybrid dynamics requires a semiclassical composition product on the classical sector*. This product is noncommutative, but the correction to the familiar classical product is small:

$$\circledast = 1 + i\hbar_C \mathcal{G} \ . \tag{4.65}$$

Recall that this does *not* require modifying the composition product for classical mechanics. What is required is the modification of the composition product for the *classical part* of hybrid variables.

Now we show that a simple construction of $\circledast$ cannot fulfil the associativity requirement, implying that this task is nontrivial. Since $\circledast$ is given by (4.16)

$$\circledast = 1 + \frac{i\hbar_C}{2}(\mathcal{P} + \sigma) \ , \tag{4.66}$$

it is completely specified by σ. If we restrict σ (like $\mathcal{P}$) to be a first-order bidifferential operator, then this symmetric product can be written as

$$\sigma(a,b,c) = a\left(\overleftarrow{\partial}_{q_C}\overrightarrow{\partial}_{q_C}\right) + b\left(\overleftarrow{\partial}_{p_C}\overrightarrow{\partial}_{p_C}\right) + c\left(\overleftarrow{\partial}_{q_C}\overrightarrow{\partial}_{p_C} + \overleftarrow{\partial}_{p_C}\overrightarrow{\partial}_{q_C}\right) \ . \tag{4.67}$$

The arbitrary parameters a, b and c define different σ-products $\sigma(a,b,c)$. For example, the σ obtained from a $\star_C$-product in the Wigner or in the Born-Jordan realization is given by $\sigma(0,0,0)$. For the Husimi realization it is $\sigma(a^2, 1/a^2, 0)$. The standard and antistandard $\star_C$ yield $\sigma(0,0,\pm 1)$. It can be shown, by direct expansion, that $\circledast$ is not associative *for general hybrid variables* for any value of (a,b,c).

This negative result implies that the simple form (4.67) is insufficient for constructing a consistent quantum-classical bracket if one insists on including all possible hybrid variables into the theory. It is unclear whether it is possible to construct a more complicated setup that achieves associativity of general variables.

This result could have a more interesting interpretation. Instead of constructing (if possible) an exotic associative product for all variables, we can read the associativity condition as imposing a *restriction* on the allowed hybrid variables. This will be explored in the next section.

4.5 Associative subalgebra of hybrid variables

The associativity of $(\star\circledast)$ guarantees that the quantum-classical bracket

$$\{\![\cdot\,,\cdot]\!\} = \frac{1}{i\hbar}\left[\star\circledast - \star^t\circledast^t\right] \tag{4.68}$$

obeys the Jacobi identity

$$\{[\{[u,v]\},w]\} + \{[\{[v,w]\},u]\} + \{[\{[w,u]\},v]\} = 0 \tag{4.69}$$

and the Leibniz rule with respect to the $(\star\circledast)$-product

$$\{[u, v \star\circledast w]\} = \{[u,v]\} \star\circledast w + u \star\circledast \{[v,w]\} \ . \tag{4.70}$$

Since $\star$ is associative, then the associativity of $(\star\circledast)$ requires the associativity of $\circledast$.

If we choose the simple form of $\circledast$

$$\circledast = 1 + \frac{i\hbar_C}{2}(\mathcal{P} + \sigma) \tag{4.71}$$

with

$$\sigma = a\left(\overleftarrow{\partial}_{q_C}\overrightarrow{\partial}_{q_C}\right) + b\left(\overleftarrow{\partial}_{p_C}\overrightarrow{\partial}_{p_C}\right) + c\left(\overleftarrow{\partial}_{q_C}\overrightarrow{\partial}_{p_C} + \overleftarrow{\partial}_{p_C}\overrightarrow{\partial}_{q_C}\right) \tag{4.72}$$

(which is motivated by $\lim_{\hbar_C^2\to 0} \star_C = \circledast$), then the associativity condition can have the following interpretation. Only a subset of all possible classical variables can be combined with any quantum variable to form a hybrid variable admissible by the theory. The minimal $\circledast$ selects classical variables $u_C(q_C, p_C)$ to form an associative subalgebra. We emphasize that hybrid dynamics admits all quantum variables and all classical variables, but restricts the classical part of *hybrid* variables, so that allowed hybrid variables take the form

$$u(q_Q, p_Q, q_C, p_C) = f(q_Q, p_Q)\ g_{\text{restricted}}(q_C, p_C) \ . \tag{4.73}$$

Since the associativity condition determines the allowed class of hybrid variables, it selects only certain interaction Hamiltonians out of infinite possibilities. Thus asso-

ciativity might be interpreted as a condition for the permissible interactions between classical and quantum systems. It is interesting when a dynamical framework determines the set of allowable theories purely on grounds of internal consistency.

As a proof of principle, we now list a few examples of associative subalgebras of $\circledast$ when σ is given by the simple expression (4.72). In the following, α, β and γ are arbitrary constants.

Example 1: For any choice of (a, b, c), the set of linear functions $f(\alpha\, q_C + \beta\, p_C)$ is associative under $\circledast$. This means that we can have consistent hybrid dynamics of any quantum variable, any classical variable, and hybrid variables that are of the form

$$u(q_Q, p_Q, q_C, p_C) = f(q_Q, p_Q)\,(\alpha\, q_C + \beta\, p_C)\ . \tag{4.74}$$

Example 2: For the case of $\sigma(0, b, c)$, the set of all functions of q_C only is allowed. So, for $\sigma(0, b, c)$, we can admit hybrid variables of the form

$$u(q_Q, p_Q, q_C) = f(q_Q, p_Q)\, g(q_C)\ . \tag{4.75}$$

Similarly, for $\sigma(a, 0, c)$ we can have

$$u(q_Q, p_Q, p_C) = f(q_Q, p_Q)\, g(p_C)\ . \tag{4.76}$$

Hybrid variables of the form (4.75) cover many interesting interaction Hamiltonians where any quantum variable is coupled to classical degrees of freedom, but not momenta. These choices for σ include ones obtained from the Wigner, Born-Jordan, standard and antistandard realizations.

Example 3: For the case of $\sigma(0, 0, \pm 1)$, all hybrid functions of the form

$$u(q_Q, p_Q, q_C, p_C) = f(q_Q, p_Q)\,(\alpha\, q_C + \beta\, p_C + \gamma\, q_C\, p_C) \tag{4.77}$$

is allowed. These two choices of σ correspond to the ones obtained from the standard and antistandard realizations, respectively.

Every choice of the $\circledast$-product selects out possible hybrid variables and, by extension, quantum-classical interaction Hamiltonians. Conversely, we can choose a certain Hamiltonian that we deem physically interesting and then find the $\circledast$-product, if any, that allows for it.

The above examples serve to show that restricting hybrid variables to certain associative subalgebras may still include interesting quantum-classical interactions. It remains to be shown if a general classification of subalgebras can be found. Importantly, it also remains to be shown how a state distribution can be constructed from such restricted hybrid variables.

4.6 Minimal subalgebra and Hamiltonian constraints

We now explore a special class of $\circledast$-associative subalgebras, ones that reduce $\circledast$ into the pointwise product of familiar classical mechanics. The use of the generally noncommutative $\circledast$ as a composition product for classical variables requires interpretation. For example, a noncommutative composition product implies the existence of a Heisenberg-like uncertainty relation. One might desire to have the advantages of hybrid dynamics while maintaining all the usual features of classical mechanics. This can be achieved by imposing further restrictions on the set of allowed hybrid variables.

Consider a subset of classical variables $f(q_C, p_C)$ such that

$$f(q_C, p_C) \circledast g(q_C, p_C) = f(q_C, p_C)\, g(q_C, p_C) \ . \tag{4.78}$$

Clearly, this subset forms an associative subalgebra with $\circledast$. For these variables, the $\circledast$-product has the same interpretation as the familiar composition product of classical

mechanics. We call this subset, along with its $\circledast$ the *minimal $\circledast$-associative subalgebra*.

Note that $\circledast$ still shows up in the Leibniz rule for the hybrid bracket as

$$\{\![u, v \star w]\!\} = \{\![u, v]\!\} \star\circledast w + u \star\circledast \{\![v, w]\!\} \ . \tag{4.79}$$

Composing the hybrid variables v and w as $(v \star\circledast w)$ yields $(v \star w)$ on the left hand side. Unless all hybrid brackets $\{\![u, v]\!\}$ belong to the same set whose classical part reduces the $\circledast$-product into the pointwise product (which is clearly too restrictive), the $\circledast$-product on the right hand side will not go away. Thus, by selecting a special class of hybrid variables, the $\circledast$-product serves as the intuitive composition product *and* preserves the consistency of the quantum-classical bracket.

To construct a minimal subalgebra, recall that $\circledast = 1 + i\hbar_C \mathcal{G}$ with $\mathcal{G} = (\mathcal{P} + \sigma)/2$, so the condition becomes $f(q_C, p_C)\, \mathcal{G}\, g(q_C, p_C) = 0$. If we choose the simple form (4.72) of σ used in the previous section, then the condition becomes

$$f \left[a \overleftarrow{\partial}_{q_C} \overrightarrow{\partial}_{q_C} + b \overleftarrow{\partial}_{p_C} \overrightarrow{\partial}_{p_C} + (c+1) \overleftarrow{\partial}_{q_C} \overrightarrow{\partial}_{p_C} + (c-1) \overleftarrow{\partial}_{p_C} \overrightarrow{\partial}_{q_C} \right] g = 0 \ . \tag{4.80}$$

This condition must also be satisfied when applied to the $\circledast$-product of a function with itself. Then, a variable $\kappa(q_C, p_C)$ belonging to the minimal subalgebra must satisfy

$$a \left(\frac{\partial \kappa}{\partial_{q_C}} \right)^2 + b \left(\frac{\partial \kappa}{\partial_{p_C}} \right)^2 + 2c \, \frac{\partial \kappa}{\partial_{q_C}} \, \frac{\partial \kappa}{\partial_{p_C}} = 0 \ . \tag{4.81}$$

We call this the self-associativity condition.

As a special case, all functions of a given solution κ of (4.81) form a minimal subalgebra with the $\circledast$-product defined by the parameters (a, b, c). To reiterate, all hybrid functions of the form

$$u(q_Q, p_Q, q_C, p_C) = f(q_Q, p_Q)\, g\big(\kappa(q_C, p_C)\big) \tag{4.82}$$

are allowed hybrid functions such that $u \star \circledast v = u \star v$ and the hybrid bracket is consistent.

An example of a minimal subalgebra obtained for all $\sigma(a, b, c)$ is the set of all functions $f(\kappa)$ such that

$$\kappa(q_C, p_C) = q_C \pm \frac{\mp c + \sqrt{c^2 - ab}}{b} p_C \ . \tag{4.83}$$

For $\sigma(s^2, 1/s^2, 0)$, obtained from the Husimi realization, we have $\kappa = q_C \pm i s^2 p_C$.

An interesting possibility arises when we examine the self-associativity condition (4.81). If we require $\kappa(q_C, p_C)$ to be nonlinear in q_C and p_C then it is possible that no choice of (a, b, c) could satisfy the equation. In that case, the condition (4.81) is one of the type

$$\phi(q_C, p_C) = 0 \ . \tag{4.84}$$

This is a *Hamiltonian constraint*. That is, minimal quantum-classical mechanics can impose geometrical constraints on the phase space of classical variables.

Constraints arise in other contexts as a consequence of certain physical symmetries such as general covariance or gauge invariance [21, 22]. Here, Hamiltonian constraints are a consequence of restricting the space of possible hybrid variables. That restriction is itself a possible requirement for the consistency of quantum-classical dynamics.

Chapter 5

Conclusion

The abstract similarity between quantum and classical algebras of observables motivates the notion that a formal structure underlies all fundamental dynamical frameworks. This structure relies on the existence of a composition product and a dynamical bracket. The dynamical bracket must satisfy the requirements of antisymmetry, linearity, Jacobi identity and the Leibniz rule with respect to the composition product.

The above requirements are necessary for a consistent canonical dynamical framework. The Jacobi identity is responsible for preserving the dynamical bracket after a transformation has taken place (Eq. (2.24)), such as time translation. The Leibniz rule is necessary for equating derivatives of variables with the dynamical bracket of these variables (see Eq. (2.7) for example), such as in the equations of motion.

Irreducible uncertainties in the measurement of pairs of variables can be imposed by adopting a noncommutative composition product as can be seen from Eq. (3.81). A form of nonlocality can be introduced through the definition (3.6) of a nonlocal composition product as well.

The properties of the bracket give rise to Noether's theorem allowing for straightforward symmetries to be implemented. Gauge and other symmetries are described through Hamiltonian constraints.

The formal dynamical structure on phase space was successfully applied to Newtonian, relativistic and quantum physics. The ubiquity of this structure and the necessity of its basic properties tempt us to impose it on all dynamical frameworks.

We would like quantum-classical dynamics to possess the same qualities.

Here we summarize the main results of this thesis. A consistent hybrid quantum-classical dynamical bracket is needed. One way to achieve that is to take a page from the quantum book and define the quantum-classical dynamical bracket (4.17) as a commutator of some product. This general bracket contains the one obtained in [11] as a special case for a particular choice of the composition product, as shown in Sec. 4.2.5. As an identity, if that product is associative then the bracket obeys the Jacobi identity and the Leibniz rule with respect to that product, just as in quantum mechanics. It is then used as a composition product.

The realization of the importance of the composition product reveals a new insight for the problem of constructing hybrid quantum-classical brackets. We are now able to view the no-go theorems in [14, 15, 16, 17, 18] in light of a single mathematical condition. It is the associativity, or lack thereof, of the hybrid composition product that makes or breaks the case for hybrid brackets: associativity = consistency. The problem now is less ambiguous, and expressed in more general terms. More options for the composition product are available for consideration, either inspired by the classical limit of phase space quantum mechanics (Sec. 4.2.2) or constructed from scratch (Sec. 4.2.3).

In principle, if a set of hybrid dynamical variables and an appropriate product form an associative algebra, then it is possible to find a way around the no-go theorem. That solution, however, is not straightforward. The no-go theorem is now generalized to forbid all simple constructions of the hybrid product (4.66) and (4.67). Using the associativity condition, we can envision two possible scenarios: construct an associative product for general variables, which is a nontrivial task, or interpret the condition as admitting only a subset of variables that are associative under a given product.

The latter of these two options, discussed in Sec. 4.5, is attractive, since it doesn't

require the introduction of complicated structures. One can choose any composition product then, using associativity as a filter, obtain a class of allowed hybrid variables. We find this interpretation of the condition interesting. It narrows down the options for allowed interactions between quantum and classical systems on the basis of consistency. Further exploration of this path leads to an interpretation of the consistency condition as a Hamiltonian constraint on the canonical variables.

It is worth noting that such restriction on admissible variables is applied only to the classical part of hybrid variables. Since the quantum product is associative by definition, all quantum variables are allowed into hybrid variables. It is the classical side that needs to be restricted (Eq. (4.73)). The "restricted variable" interpretation of the consistency condition then does not fully treat quantum and classical systems on equal footing.

A special condition can be imposed on the framework motivated by arguments of simplicity. The composition product(s) (4.66) introduced for classical variables is noncommutative and contains $\hbar$. It can be viewed as a semiclassical approximation to a full quantum product or, equivalently, as a first order quantum correction to the pointwise multiplication of standard classical mechanics. One can take a conservative approach and require the choice of subalgebra that reduces composition product of its elements to pointwise multiplication (Eq. (4.78)). That way, the composition of classical variables retain the familiar meaning while simultaneously allowing for the construction of a consistent hybrid dynamics. We consider this a minimal setup for quantum-classical dynamics in Sec. 4.6. The term is inspired by the concept of minimal coupling in general relativity, the procedure by which one obtains the simplest general theory from a less general one.

The analysis presented here invites exploration of interesting possibilities. More work remains to be done and questions to be answered. Can a general associative product be constructed for all classical variables? What nontrivial setup would be

needed for that, and what would it imply for classical mechanics and its relation to quantum mechanics? On the other hand, if we choose to restrict hybrid variables to an associative subalgebra, can we find a general classification of these subalgebras? How can we interpret the relationship between different composition products and the interactions they allow for? Further, the Hamiltonian constraints (4.84) need to be studied in detail to fully understand their implications and relation to gauge symmetries.

An important ingredient in the quantum-classical framework that has been left for future study is the state distribution. The state is treated differently in quantum than in classical mechanics, what constitutes a meaningful quantum-classical state distribution? In the case of restricted hybrid variables, can a state distribution be constructed from these variables? What are the equations of motion for the reduced distributions on the quantum and classical sectors? What can quantum-classical dynamics say about the quantum state collapse?

Other aspects of dynamics should be explored as well. For example, what are the allowed hybrid transformations and symmetries? Can the results be translated into other formulations, like the Lagrangian formulation? How can consistent quantum-classical statistical mechanics be formulated?

After these fundamental questions have been answered, we can move on to explore applications of the quantum-classical framework to interesting physical situations. Examples may include applications in condensed matter physics, chemical physics early universe cosmology and gravitational singularities.

The current proposal offers a new perspective on the problem of quantum-classical dynamics. Further investigation will test its effectiveness and reveal its implications. Exciting possibilities lie ahead.

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