From classical to quantum mechanics (and back)

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Abstract

These lecture notes are addressed to PhD students in mathematical physics and applied geometric mechanics. After presenting Koopman's Hilbert space formulation of classical mechanics and its connections to prequantization theory, the basic notions of quantum mechanics are introduced by making use of standard techniques in geometric mechanics, such as the Hopf bundle, group orbits and momentum maps. In the last part, this construction is applied to mixed classical-quantum dynamics as it emerges in chemical physics problems. After the Euler-Poincaré formulation of the Ehrenfest mean-field model, the geometry of expectation value dynamics is unfolded in terms of semidirect-product Lie groups. This construction produces the energy-conserving variant of a class of models previously appeared in the chemical physics literature.

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1.1 The classical Liouville equation

At the heart of classical mechanics lies the Liouville equation for probability density functions on a symplectic manifold (M, ω). If we denote by $\rho(z, t)$ a (time-dependent) probability density function on $M \ni z$, the (classical) Liouville equation reads

$$\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0$$

Here, $\{\cdot, \cdot\}$ is the Poisson bracket induced by the symplectic form ω, while $H(z) \in C^\infty(M)$ is the Hamiltonian of the system under consideration.

In physics, the Liouville density contains the statistical information on the physical system under consideration. More specifically, we are in a situation in which we have no exact information on the particle trajectory (in the simplest case of one-particle systems). Rather, the quantity $\rho(z, t)$ is a probabilty distribution for the particle phase-space coordinate. For example, if we are interested in the particle momentum p, the only information we can extract is the *expectation value* at the time t:

$$\langle p \rangle(t) = \int_M p\rho(z, t)\, \mathrm{d}^{2n}z$$

The particle trajectory on phase-space, as described by $(\bar{q}(t), \bar{p}(t))$, is only recovered in the special case of a delta function solution

$$\rho(z, t) = \delta(z - \bar{z}(t))\,.$$

Indeed, replacing the above (weak) solution ansatz and taking the pairing with a test function yields Hamilton's equations $\dot{z} = \{\bar{z}, H(\bar{z})\}$. Then, the Liouville equation captures all features of classical mechanics. Even more, we can identify classical mechanics with the Liouville equation! This picture is particularly suggestive in bridging across with quantum mechanics.

1.2 Geometric structure

The Liouville equation has an intrinsic geometric structure. For example, we can exploit the relation $\pounds_{X_F} G = X_F(G) = \{G, F\}$. Here, $\pounds$ denotes Lie derivative, while X_F denotes a Hamiltonian vector field with Hamiltonian $F(z)$. Then, we can rewrite the Liouville equation as

$$\frac{\partial \rho}{\partial t} + \pounds_{X_H}\rho = 0\,. \tag{1}$$

Notice that we have identified densities with scalar functions: this is possible since once can write $\rho = \bar{\rho}\mu$, where $\bar{\rho}$ is a scalar function and μ is the Liouville volume such that $\pounds_{X_H}\mu = 0$.

Actually, the Liouville equation is a Lie-Poisson system on the Poisson (Lie) algebra of Hamiltonian functions

$$\mathfrak{g} = C^\infty(\mathbb{R}^{2n})$$

To see this, consider the functional

$$h[\rho] = \int_M \rho\, H\,,$$

so that

$$\frac{\delta h}{\delta \rho} = H.$$

Here, $\delta h/\delta\rho$ is a functional derivative such that

$$\delta h = \int_M \frac{\delta h}{\delta \rho}\,\delta\rho\,,$$

where δh is defined as

$$\delta h := \lim_{\epsilon\to 0}\frac{h[\rho+\epsilon\delta\rho]-h[\rho]}{\epsilon}\,.$$

At this point, we can take another arbitrary functional $f[\rho]$ and compute its time derivative as follows

$$\dot f[\rho] = \int_M \frac{\delta f}{\delta\rho}\frac{\partial\rho}{\partial t} = \int_M \frac{\delta f}{\delta\rho}\left(-\pounds_{X_{\delta h/\delta\rho}}\rho\right) = \int_M \rho\left(\pounds_{X_{\delta h/\delta\rho}}\frac{\delta f}{\delta\rho}\right) = \int_M \rho\left\{\frac{\delta f}{\delta\rho},\frac{\delta h}{\delta\rho}\right\} =: \{f,h\}[\rho]\,.$$

Then, we have shown that the Liouville equation possesses a Lie-Poisson bracket on the Poisson (Lie) algebra of Hamiltonian functions. Thus, from the theory of Lie-Poisson reduction, ρ evolves under the coadjoint representation as

$$\rho(t) = \mathrm{Ad}^*_{\eta^{-1}}\rho(0)$$

But what is the group underlying this Poisson algebra? What is η really? More specifically, we look for a group G such that

$$T_eG = \mathfrak{g} = C^\infty(\mathbb{R}^{2n})$$

We shall discuss this important point later. For now, we observe that the equation (1) allows us to write

$$\rho(t) = \eta_*(t)\rho(0)\,,$$

where η_* denotes the push-forward of ρ by the Hamiltonian flow $\eta(t)$ generated by the Hamiltonian vector field X_H. More explicitly, we have the *Lagrange-to-Euler map*

$$\rho(z,t) = (\eta(t)_*\rho_0)(z) = \int_M \rho_0(z_0)\,\delta(z-\eta(z_0,t))\,\mathrm{d}^{2n}z_0\,.$$

A direct calculation shows that taking the time derivative of the relation above returns indeed (1).

Thus, we are led to the idea that the Liouville equation identifies coadjoint orbits on the group of canonical transformations such that

$$\eta^*\omega = \omega\,.$$

However, things are actually more complicated than that, as we shall see.

1.3 Koopman-von Neumann approach

In 1931, Bernard Koopman [21] (and one year later von Neumann [35]) gave classical mechanics a Hilbert space description, which has attracted some attention only recently [6]. Here, we restrict our attention to the simplest case $(M,\omega) = (\mathbb{R}^{2n},\mathbb{J})$, where $\mathbb{J}$ denotes the canonical symplectic form.

One introduces the Hilbert space

$$\mathscr{H} = L^2(\mathbb{R}^{2n})$$

and look for solutions of the Liouville equation of the form

$$\rho(z,t) = |\psi(z,t)|^2\,, \qquad \text{with} \qquad \psi \in \mathscr{H}\,.$$

In analogy with quantum mechanics, ψ is called the *probability amplitude* for the Liouville probability density. For example, given a physical observable represented by a phase-space function $A(z)$ (e.g. the magnitude of the angular momentum $|q \times p|$), its classical expectation value is now computed as

$$\langle A\rangle(t) = \int \rho(z,t)A(z)\,\mathrm{d}^{2n}z = \int \psi^*(z,t)A(z)\psi(z,t)\,\mathrm{d}^{2n}z = \langle\psi|A\psi\rangle\,,$$

where we have defined the Hermitian inner product

$$\langle\psi_1|\psi_2\rangle := \int \psi_1^*(z,t)\psi_2(z,t)\,\mathrm{d}^{2n}z\,.$$

By direct verification, Koopman noticed that

$$\frac{\partial\psi}{\partial t} = \{H,\psi\}$$

returns the Liouville equation for $\rho(z,t) = |\psi(z,t)|^2$. This is proved by Leibniz rule:

$$\frac{\partial|\psi|^2}{\partial t} = (\partial_t\psi^*)\psi + \psi^*\partial_t\psi = \{H,\psi^*\}\psi + \psi^*\{H,\psi\} = \{H,|\psi|^2\} - \psi^*\{H,\psi\} + \psi^*\{H,\psi\} = \{H,|\psi|^2\}$$

Then, one can formally write the solution for ψ as

$$\psi(t) = \eta_*\psi_0\,.$$

Since the pushforward is a linear action (representation) and we have just proved that

$$\|\psi(t)\|^2 = \|\psi(0)\|^2 = \int_M \rho = 1\,,$$

then

Theorem 1.1 (Koopman (1931)) *The action of symplectic diffeomorphisms*

$$\mathrm{Symp}(\mathbb{R}^{2n}) = \{\eta \in \mathrm{Diff}(\mathbb{R}^{2n})\,|\,\eta^*\omega = \omega\}$$

on the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^{2n})$ *is a unitary representation.*

While this result is widely used in ergodic theory (Koopmanism is actually a branch of this discipline), this observation can serve as the beginning for a series of speculations about similarities between quantum and classical dynamics. Indeed, we know that unitary transformations are the essential ingredient of classical mechanics.

1.4 The Liouvillian operator

As we shall see, Koopman's probability amplitudes obey very similar equations to those of quantum mechanics. To see this, let's rewrite the probability amplitude equation as

$$i\frac{\partial\psi}{\partial t} = \{iH,\psi\} = i\nabla H\cdot\mathbb{J}\nabla\psi = (\mathbb{J}\nabla H)\cdot(-i\nabla\psi) = \kappa^{-1}X_{H}\cdot(-i\kappa\nabla\psi)\,,$$

where the $X_H(\mathbf{z}) = \mathbb{J}\nabla H(\mathbf{z})$ is the Hamiltonian vector field for H and the constant κ is introduced for later convenience. At this point, we introduce the Hermitian operators $(\widehat{\mathcal{Z}},\widehat{\Lambda})$ on $\mathscr{H}$ as follows [6, 32]:

$$(\widehat{\mathcal{Z}}\psi)(z) := z\psi(z)\,, \qquad\qquad (\widehat{\Lambda}\psi)(z) := -i\kappa\nabla\psi(z)\,.$$

Remarkably, we notice that their commutators satisfy

$$[\widehat{\mathcal{Z}},\widehat{\Lambda}] = i\kappa\mathbf{1}\,, \qquad\qquad [\widehat{\mathcal{Z}}^i,\widehat{\mathcal{Z}}^j] = [\widehat{\Lambda}_i,\widehat{\Lambda}_j] = 0\,,$$

where $\mathbf{1}$ denotes the identity matrix on $\mathbb{R}^{2n}$. Indeed, we have

$$\widehat{\mathcal{Z}}\widehat{\Lambda}\psi - \widehat{\Lambda}\widehat{\mathcal{Z}}\psi = z(-i\kappa\nabla\psi) - (-i\kappa\nabla)(z\psi) = i\kappa\psi\nabla z = i\kappa\psi\,.$$

Formally, we can define the Hermitian ***Liouvillian operator***

$$\widehat{L} = X_H(\widehat{\mathcal{Z}})\cdot\widehat{\Lambda}$$

and write the ***Koopman equation*** for the ***classical wavefunction*** as

$$i\kappa\frac{\partial\psi}{\partial t} = \widehat{L}(\widehat{\mathcal{Z}},\widehat{\Lambda})\psi\,.$$

Those who know quantum mechanics will have certainly noticed the stricking analogy with the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \widehat{H}(\widehat{Q},\widehat{P})\psi$$

for wavefunctions $\psi(x)\in L^2(\mathbb{R}^3)$. Notice that, in order to describe a mechanical system the Liouvillian must be of the form $X_H(\widehat{\mathcal{Z}})\cdot\widehat{\Lambda}$, while the Hamiltonian operator $\widehat{H}(\widehat{Q},\widehat{P})$ can have a general form in quantum mechanics.

1.5 Van Hove's result and Souriau's quantomorphism group

So far, everything seems clear: classical wavefunctions evolve on orbits of the symplectic diffeomorphisms. However, we notice that there are infinitely many possible wavefunctions returning the same Liouville density. Indeed, any phase-type transformation

$$\psi(z)\mapsto e^{i\varphi(z)}\psi(z)$$

leaves the Liouville density $|\psi(z)|^2$ invariant (here $\varphi\in C^\infty(\mathbb{R}^{2n},S^1)$). In addition, in 1951 Van Hove [34] noticed that the representation of symplectic diffeomorphisms on classical wavefunctions is not faithful. We recall that a group $G-$action $\Phi_g : M\to M$ on M is faithful iff

$$\Phi_g = \mathrm{Id} \implies g = e\,,$$

where e denotes the identity group element. That is, the group representation is one-to-one.

In the preceding sections, we always focused our attention on canonical transformations (or, equivalently, symplectic diffeomorphisms) because we saw that they emerge naturally in the study of the Liouville equation. In our analysis of equation (1), we considered the symplectic diffeomorphism η generated by the Hamiltonian vector field X_H and we were led to think that the Lie group underlying the Lie-Poisson structure of the Liouville equation is the group of symplectic diffeomorphisms. However, the latter has as its Lie algebra the space of Hamiltonian vector fields

$$T_e\text{Symp}(\mathbb{R}^{2n}) = \mathfrak{X}_{\text{Ham}}(\mathbb{R}^{2n})\,,$$

which we know is homomorphic to the Poisson algebra of Hamiltonian functions since

$$[X_F, X_H] = -X_{\{F,G\}}\,.$$

(Here, $\mathfrak{X}_{\text{Ham}}(\mathbb{R}^{2n})$ denotes the Lie algebra of Hamiltonian vector fields and $[X_F, X_H]$ denotes the Jacobi-Lie bracket on vector fields). On the other hand, the two Lie algebras

$$\mathfrak{X}_{\text{Ham}}(\mathbb{R}^{2n}) \qquad\qquad C^\infty(\mathbb{R}^{2n})$$

are *not* isomorphic. Indeed, Hamiltonians are only defined up to constants and one can see that upon considering the quotient space $C^\infty(\mathbb{R}^{2n})/\mathbb{R}$, one has

$$\mathfrak{X}_{\text{Ham}}(\mathbb{R}^{2n}) \simeq C^\infty(\mathbb{R}^{2n})/\mathbb{R}\,.$$

Thus, we need to add extra structure to the group of symplectic diffeomorphisms if we want to recover the Poisson algebra of Hamiltonian functions.

The diffeomorphism group possessing the space of Hamiltonian functions as its Lie algebra was treated by Van Hove in his thesis. In 1968, this name was given the name of ***quantomorphism group*** by Jean-Marie Souriau [31], as it emerges in geometric quantization. In its modern formulation, this is constructed as a central extension of the symplectic diffeomorphisms by the real numbers. The group multiplication on

$$\text{Quant}(\mathbb{R}^{2n}) = \text{Symp}(\mathbb{R}^{2n}) \times \mathbb{R}$$

reads

$$(\eta_1, c_1)(\eta_2, c_2) = \left(\eta_1 \circ \eta_2,\, c_1 + c_2 + \int_0^{\eta_2(0)} (\eta_1^*\mathcal{A} - \mathcal{A})\right)\,,$$

where $\mathcal{A}$ is the canonical one-form on $T^*\mathbb{R}^n = \mathbb{R}^{2n}$ (e.g. $A(z)\cdot \mathrm{d}z = p\mathrm{d}q$) and the integral is taken along a smooth curve connecting the origin to $\eta_2(0)$ (one can prove that this integral is independent of the choice of curve). This definition can be generalized easily to exact symplectic manifolds (as long as $H^1(M,\mathbb{R}) = 0$), although we shall not go there.

The quantomorphism action on classical wavefunctions reads

$$(\eta, c) : \psi(z) \mapsto e^{-\frac{i}{\kappa}\left(c + \int_0^z (\eta^*\mathcal{A} - \mathcal{A})\right)}(\eta^*\psi)(z)\,,$$

where we recognize the (carefully chosen!) phase terms in the action. In his thesis, Van Hove proved that this action is faithful for any value of κ, thereby allowing for improvements in Koopman's theory.

After this digression into the basics of geometric quantization, we shall leave the Koopman framework to look at its Schrödinger counterpart in quantum mechanics.

2 Geometric introduction to quantum mechanics

2.1 Pure quantum states and the Schrödinger equation

Koopman's theory has provided a framework in which classical mechanics can be expressed in terms of dynamics on a Hilbert space. In turn, this is precisely what happens in quantum mechanics, where a *pure quantum state* is defined by a unit vector ψ in a complex Hilbert space $\mathscr{H}$. The fundamental equation of quantum mechanics is Schrödinger's equation, which reads

$$i\hbar\dot{\psi} = \widehat{H}\psi\,. \tag{2}$$

Here, $\hbar$ is a constant (Planck's constant), the dot denotes a time derivative and the linear Hermitian operator $\widehat{H}$ is called ***Hamiltonian operator***. Here, we shall only consider Hamiltonian operators that do not depend explicitly on time.

Since it is a linear equation, Schrödinger's equation is formally solved directly as

$$\psi(t) = e^{-\frac{i}{\hbar}\widehat{H}t}\psi(0)$$

where the exponential $e^{-\frac{i}{\hbar}\widehat{H}t}$ is known in physics as the ***propagator***. This operator is actually unitary, that is

$$U(t) = e^{-\frac{i}{\hbar}\widehat{H}t} \in \mathcal{U}(\mathscr{H})\,,$$

where

$$\mathcal{U}(\mathscr{H}) = \{U \in L(\mathscr{H})\,|\,UU^\dagger = \mathbf{1}\}$$

denotes the group of unitary operators on the Hilbert space $\mathscr{H}$. (Here, $U^\dagger$ denotes the adjoint operator of U with respect to the Hermitian inner product on $\mathscr{H}$; in infinite dimensions, one asks for U to be bounded). The emergence of the unitary group in quantum mechanics confers the theory a non-trivial geometric significance.

While in classical mechanics physical observables are represented by phase-space functions $A(z)$, in quantum mechanics, they are represented by Hermitian operators $\widehat{A}$. Similarly to Koopman mechanics, their expectation values are computed by using the Hermitian inner product on $\mathscr{H}$, that is

$$\langle\widehat{A}\rangle(t) = \langle\psi(t)|\widehat{A}\psi(t)\rangle\,.$$

Their equation of motion was found in Ehrenfest in 1927 [12] by simply using the Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\widehat{A}\rangle = i\hbar^{-1}\langle\psi|[\widehat{H},\widehat{A}]\psi\rangle = i\hbar^{-1}\langle[\widehat{H},\widehat{A}]\rangle \tag{3}$$

As we shall see, expectation values play a crucial role in quantum mechanics. Their momentum map features will be unfold in the next sections.

2.2 Finite vs. infinite dimensions and Heisenberg's uncertainty

So far, nothing has been said about the dimension of the Hilbert space $\mathscr{H}$. In the simplest case (which is particularly relevant in practical applications), one has $\mathscr{H} = \mathbb{C}^n$ and the Hamiltonian operator (as well as the other observables) are simply $n \times n$ complex matrices. In infinite dimensions (which is the more realistic case), one deals with the infinite-dimensional Hilbert space

$$\mathscr{H} = L^2(\mathbb{R}^3)\,.$$

In this case, the unit vector ψ is a normalized ***wavefunction*** $\psi(x,t)$ (such that $\|\psi\|^2 = 1$) and the Hamiltonian operator is a function of two operators called ***canonical observables*** and denoted by $(\widehat{Q}, \widehat{P})$. These operators satisfying the ***canonical commutation relations***

$$[\widehat{Q}, \widehat{P}] = i\hbar\mathbf{1}\,, \qquad\qquad [\widehat{Q}^i, \widehat{Q}^j] = [\widehat{P}^i, \widehat{P}^j] = 0\,. \tag{4}$$

(Notice that the first relation would not make sense in finite dimensions, since in that case $\mathrm{Tr}[\widehat{A}, \widehat{B}] = 0$). In standard formulations of quantum mechanics the Hamiltonian is of the type $\widehat{H} = \widehat{H}(\widehat{Q}, \widehat{P})$, and the canonical observables are written as

$$(\widehat{Q}\psi)(x) := x\psi(x)\,, \qquad\qquad (\widehat{P}\psi)(x) := -i\hbar\nabla\psi(x)\,. \tag{5}$$

The analogy with Koopman's classical mechanics appears now explicit. In problems of physical interest, the Hamiltonian operator is written as

$$\widehat{H}(\widehat{Q}, \widehat{P}) = \frac{1}{2}\widehat{P}^2 + V(\widehat{Q})\,,$$

where $V \in C^\infty(\mathbb{R}^3)$ is a real-valued physical potential.

In infinite-dimensions, convergence problems emerge, especially because the canonical observables are unbounded operators. However, here we shall assume that their expectation values always exist, along with the expectation values of all other observables. Importantly, we shall assume that all expectation values converge in the following theorem:

Theorem 2.1 (Heisenberg (1927)) *Consider two Hermitian operators $\widehat{A}$ and $\widehat{B}$. For any wavefunction $\psi(x)$, one has*

$$\sqrt{\langle(\widehat{A} - \langle\widehat{A}\rangle)^2\rangle}\sqrt{\langle(\widehat{B} - \langle\widehat{B}\rangle)^2\rangle} \geq \frac{1}{2}|\langle[\widehat{A}, \widehat{B}]\rangle|$$

Proof. For $\lambda \in \mathbb{R}$, define the non-Hermitian operator

$$\widehat{F} = \widehat{A} + i\lambda\widehat{B}$$

and introduce the function

$$\phi = \widehat{F}\psi\,.$$

Then, we compute

$$0 \leq \|\phi^2\| = \langle(\widehat{A} + i\lambda\widehat{B})^2\rangle = \langle\widehat{A}^2\rangle + \lambda\langle i[\widehat{A}, \widehat{B}]\rangle + \lambda^2\langle\widehat{B}^2\rangle$$

whose minimum is at

$$\lambda_0 = -\frac{1}{2}\frac{\langle i[\widehat{A}, \widehat{B}]\rangle}{\langle\widehat{B}^2\rangle}\,,$$

where we recall that $[\widehat{A}, \widehat{B}]$ is skew-Hermitian so that $\langle i[\widehat{A}, \widehat{B}]\rangle \in \mathbb{R}$. Evaluating $\|\phi\|^2$ at λ_0 yields

$$0 \leq \langle\widehat{A}^2\rangle - \frac{1}{2}\frac{\langle i[\widehat{A}, \widehat{B}]\rangle^2}{\langle\widehat{B}^2\rangle} + \frac{1}{4}\frac{\langle i[\widehat{A}, \widehat{B}]\rangle^2}{\langle\widehat{B}^2\rangle^2}\langle\widehat{B}^2\rangle = \langle\widehat{A}^2\rangle - \frac{i^2}{4}\frac{\langle[\widehat{A}, \widehat{B}]\rangle^2}{\langle\widehat{B}^2\rangle} = \langle\widehat{A}^2\rangle + \frac{1}{4}\frac{\langle[\widehat{A}, \widehat{B}]\rangle^2}{\langle\widehat{B}^2\rangle}$$

so that

$$\langle\widehat{A}^2\rangle\langle\widehat{B}^2\rangle \geq -\frac{1}{4}\langle[\widehat{A},\widehat{B}]\rangle^2 .$$

Now, since $\langle[\widehat{A},\widehat{B}]\rangle$ is purely imaginary and

$$[\widehat{A},\widehat{B}] = [\widehat{A} - \langle\widehat{A}\rangle, \widehat{B} - \langle\widehat{B}\rangle] ,$$

we can make the replacement

$$\widehat{A} \to \widehat{A} - \langle\widehat{A}\rangle , \qquad\qquad \widehat{B} \to \widehat{B} - \langle\widehat{B}\rangle$$

to write

$$\langle(\widehat{A} - \langle\widehat{A}\rangle)^2\rangle\langle(\widehat{B} - \langle\widehat{B}\rangle)^2\rangle \geq \frac{1}{4}|\langle[\widehat{A},\widehat{B}]\rangle|^2$$

Then, the theorem is proved by taking the square root on both sides. ■

This theorem lies at the heart of the physical interpretation of quantum mechanics. When it is specialized to the case of canonical observables, one obtains the celebrated uncertainty relation

$$\sqrt{\langle(\widehat{Q} - \langle\widehat{Q}\rangle)^2\rangle}\sqrt{\langle(\widehat{P} - \langle\widehat{P}\rangle)^2\rangle} \geq \frac{1}{2}|\langle[\widehat{Q},\widehat{P}]\rangle| = \frac{\hbar}{2}$$

which indicates that no simultaneous exact information can be achieved on both the position and momentum of the particle. On other words, we will never know exactly at what point of phase-space the particle is located.

Corollary 2.2 (Uncertainty in Koopman dynamics) *If $(\widehat{\mathscr{Z}},\widehat{\Lambda})$ are the canonical operators from Koopman's theory and ψ is any classical wavefunction, then*

$$\sqrt{\langle(\widehat{\mathscr{Z}} - \langle\widehat{\mathscr{Z}}\rangle)^2\rangle}\sqrt{\langle(\widehat{\Lambda} - \langle\widehat{\Lambda}\rangle)^2\rangle} \geq \frac{1}{2}|\langle[\widehat{\mathscr{Z}},\widehat{\Lambda}]\rangle| = \frac{\kappa}{2} .$$

Now, since in classical mechanics we have exact information about the particle location in phase-space, in 1976 this result has led Sudarshan [32] to invoke the principle by which the operators $\widehat{\Lambda}$ are *unobservable*. However, this point have never been made clear on a solid mathematical footing.

2.3 Hamiltonian formulation

It is well known that the Schrödinger equation possesses a Hamiltonian structure on $\mathscr{H}$, with (constant) symplectic form defined as (see e.g. [8])

$$\omega(\psi,\psi') = 2\hbar\,\text{Im}\langle\psi|\psi'\rangle ,$$

which in turn produces the Poisson bracket

$$\{f,h\}[\psi] = \frac{1}{2\hbar}\,\text{Im}\left\langle\frac{\delta f}{\delta\psi}\middle|\frac{\delta h}{\delta\psi}\right\rangle$$

Interestingly enough, we have the following result when we evaluate this Poisson bracket on expectation values

Proposition 2.3 *Let $(\widehat{A},\widehat{B})$ be any two Hermitian operators and consider their expectation values. One has*

$$\{\langle\widehat{A}\rangle,\langle\widehat{B}\rangle\} = \frac{1}{i\hbar}\langle[\widehat{A},\widehat{B}]\rangle .$$

Proof. We compute
$$\frac{\delta}{\delta\psi}\langle\widehat{A}\rangle = \frac{\delta}{\delta\psi}\langle\psi|\widehat{A}\psi\rangle = 2\widehat{A}\psi$$
and analogously for $\widehat{B}$. Then, we evaluate
$$\{\langle\widehat{A}\rangle,\langle\widehat{B}\rangle\} = \frac{2}{\hbar}\,\mathrm{Im}\langle\widehat{A}\psi|\widehat{B}\psi\rangle = \frac{1}{i\hbar}(\langle\widehat{A}\psi|\widehat{B}\psi\rangle - \langle\widehat{B}\psi|\widehat{A}\psi\rangle) = \langle\psi|[\widehat{A},\widehat{B}]\psi\rangle\,,$$
where we have used
$$\langle\widehat{A}\psi|\widehat{B}\psi\rangle = \int(\widehat{A}\psi)^*\widehat{B}\psi = \int\psi^*\widehat{A}^\dagger\widehat{B}\psi = \int\psi^*\widehat{A}\widehat{B}\psi = \langle\psi|\widehat{A},\widehat{B}\psi\rangle$$
and analogously for $\langle\widehat{B}\psi|\widehat{A}\psi\rangle$. Then, the proof is complete. ■

It is obvious that all these relations hold exactly the same for Koopman's classical mechanics.

2.4 Variational principles

We now look at the variational structure. Since $\mathscr{H}$ is a vector space, we can simply apply a basic result from the theory of Hamiltonian systems

Proposition 2.4 *Let (V,Ω) be a symplectic vector space. Then, Hamilton's equations*
$$\dot{z} = X_H(z)\,, \qquad\qquad \mathrm{i}_{X_H}\Omega = \mathrm{d}H$$
are equivalent to the Euler-Lagrange equations for the following degenerate Lagrangian $L : TV \to \mathbb{R}$
$$L(z,\dot{z}) = \frac{1}{2}\Omega(\dot{z},z) - H(z)\,.$$

Proof. We compute
$$\delta L = \frac{1}{2}\Omega(\dot{z},\delta z) + \frac{1}{2}\Omega(\delta\dot{z},z) - \left\langle\frac{\delta H}{\delta z},\delta z\right\rangle = \frac{1}{2}\langle\Omega^\flat(\dot{z}),\delta z\rangle - \frac{1}{2}\langle\Omega^\flat(z),\delta\dot{z}\rangle - \left\langle\frac{\delta H}{\delta z},\delta z\right\rangle\,,$$
where we have defined the flat isomorphism
$$\Omega^\flat : V \to V^*$$
induced by the symplectic form. Then, the Euler-Lagrange equations read
$$\Omega^\flat(\dot{z}) = -\frac{\delta H}{\delta z}\,.$$
Then, if we define the Lagrangian vector field $Z \in \mathfrak{X}(V)$ such that $\dot{z} = Z(z)$ and $\Omega^\flat(Z) = -\mathrm{i}_Z\Omega$, the above relation is rewritten equivalently as
$$\mathrm{i}_Z\Omega = \mathrm{d}H$$
so that
$$Z = X_H$$

and the proof is complete. ■

A simple adaptation of this theorem yields the celebrated Dirac-Frenkel (DF) Lagrangian for the Schrödinger equation

$$L(\psi,\dot\psi)=\hbar\,\mathrm{Im}\langle\dot\psi|\psi\rangle-h(\psi)\,,\qquad\text{with}\qquad h(\psi)=\langle\psi|\widehat{H}\psi\rangle\,.$$

It is convenient to rewrite this in terms of the ***non-degenerate real-valued pairing***

$$\langle\psi_1,\psi_2\rangle:=\mathrm{Re}\langle\psi_1|\psi_2\rangle=\mathrm{Re}(\psi_1^\dagger\psi_2)\,,$$

where we notice that

$$\langle i\psi_1,\psi_2\rangle=\frac{1}{2}(\langle i\psi_1|\psi_2\rangle+\overline{\langle i\psi_1|\psi_2\rangle})=-\frac{i}{2}(\langle\psi_1|\psi_2\rangle-\overline{\langle\psi_1|\psi_2\rangle})=\mathrm{Im}\langle\psi_1|\psi_2\rangle$$

and thus, the DF Lagrangian becomes

$$L(\psi,\dot\psi)=\hbar\,\langle\psi,i\dot\psi\rangle-h(\psi)\,,\qquad\text{with}\qquad h(\psi)=\langle\psi|\widehat{H}\psi\rangle\,,$$

since $\langle\psi_1,\psi_2\rangle=\langle\psi_2,\psi_1\rangle$.

Corollary 2.5 (Dirac & Frenkel (1934) [11, 13]) *The Schrödinger equation (2) arises as the Euler-Lagrange equation of the Lagrangian*

$$L(\psi,\dot\psi)=\hbar\,\langle\psi,i\dot\psi\rangle-\langle\psi|\widehat{H}\psi\rangle\,. \tag{6}$$

Proof. Upon using $\langle i\psi_1,\psi_2\rangle=-\langle\psi_1,i\psi_2\rangle$, taking variations yields

$$\delta L=\hbar\,\langle i\dot\psi,\delta\psi\rangle-\hbar\,\langle i\psi,\delta\dot\psi\rangle-2\langle\widehat{H}\psi,\delta\psi\rangle\,,$$

so that the Euler-Lagrange equations return

$$-2i\hbar\dot\psi+2\widehat{H}\psi=0\,.$$

Then, the proof is complete ■

We conclude by noticing (again!) that all the discussion in this section goes through in Koopman's classical mechanics upon replacing the Hamiltonian operator $\widehat{H}$ by the Liouvillian $\widehat{L}$. This comes as no surprise, since we have already seen how the two theories share several geometric properties.

2.5 Normalization and phases: the Hopf bundle

So far, we always worked on the Hilbert space $\mathscr{H}$ without ever including the normalization condition

$$\|\psi\|^2=1$$

explicitly. This normalization condition amounts to saying that the total probability of finding one particle within the entire system is 1. A natural way of including this normalization condition would be to work on the unit sphere

$$S(\mathscr{H})=\{\psi\in\mathscr{H}\,|\,\|\psi\|^2=1\}\,.$$

Technically, this would require working on a manifold, that is possibly infinite dimensional [9]. A simpler way of approaching the problem is to use a constraint in the DF Lagrangian, which then becomes

$$L(\psi, \dot{\psi}, \phi, \dot{\phi}) = \hbar \langle \psi, i\dot{\psi} \rangle - \langle \psi | \widehat{H}\psi \rangle + \nu(1 - \|\psi\|^2)\,.$$

The corresponding Euler-Lagrange equations read

$$i\hbar\dot{\psi} = \widehat{H}\psi + \nu\psi\,, \tag{7}$$

along with the normalization condition. Now, pairing with ψ yields

$$\nu = \hbar\langle \psi, i\dot{\psi} \rangle - \langle \psi, \widehat{H}\psi \rangle$$

and thus the equation becomes

$$i\hbar\dot{\psi} = \widehat{H}\psi + \langle \psi, i\hbar\dot{\psi} - \widehat{H}\psi \rangle\psi\,. \tag{8}$$

This is Schrödinger equation on the unit sphere $S(\mathscr{H})$.

In his work [19], the author considered the equation (7) with the important difference of letting $\nu \in \mathbb{R}$ be an arbitrary time-dependent parameter. The reason for letting λ be arbitrary is that its presence does not affect any of the quantities with physical meaning. Indeed, the expectation value equation (3) are totally insensitive with respect to the replacement $\widehat{H} \to \widehat{H} + \nu\mathbf{1}$, because the identity commutes with all linear operators in $L(\mathscr{H})$. Now, if we look at the solutions of equation (7), upon introducing $\varphi(t)$ such that $\dot{\varphi}(t) = \nu(t)$ we have

$$\psi(t) = e^{-i\hbar(\widehat{H}t + \varphi(t)\mathbf{1})}\psi(0)\,.$$

Thus, the unitary transformation producing the $\nu-$term in (7) is a (phase) transformation of the type

$$\psi \mapsto e^{-i\hbar\varphi}\psi\,,$$

which identifies the action of the Abelian Lie group S^1, that is the circle group. One calls this action of S^1 on the Hilbert space $\mathscr{H}$ a ***phase transformation***, so that the circle group is regarded as the group of phase transformations and is denoted by $\mathcal{U}(1)$. It is important to notice the following

Proposition 2.6 (Phase-invariance) *The DF Lagrangian (6) is invariant under the tangent lifts of the $\mathcal{U}(1)-$action on $\mathscr{H}$ given by*

$$\psi \mapsto e^{-i\hbar\varphi}\psi\,.$$

Proof. *The tangent lifts of phase transformations are easily computed from the definition as*

$$(\psi, \dot{\psi}) \mapsto (e^{-i\hbar\varphi}\psi, e^{-i\hbar\varphi}\dot{\psi})\,.$$

Then, since $[\widehat{H}, e^{-i\hbar\varphi}\mathbf{1}] = 0$, we have

$$\langle e^{-i\hbar\varphi}\psi | \widehat{H} e^{-i\hbar\varphi}\psi \rangle = \langle \psi | \widehat{H}\psi \rangle$$

In addition, we have

$$\langle e^{-i\hbar\varphi}\psi, ie^{-i\hbar\varphi}\dot{\psi} \rangle = \langle \psi, i\dot{\psi} \rangle$$

and thus the proof is complete. ■

Since we have discussed how phases are irrelevant to physical quantities, we want to identify all unit vectors in $\mathscr{H}$ that differ by a phase, so that $\psi \sim e^{-i\hbar\varphi}\psi$. That is, we want to consider elements (equivalence classes) of the quotient space $S(\mathscr{H})/S^1$ or, equivalently,

$$S(\mathscr{H})/\mathcal{U}(1) = \mathbf{P}\mathscr{H}\,,$$

which is called the ***projective Hilbert space***. A convenient way of defining the elements of $\mathbf{P}\mathscr{H}$ is by the definition

$$\mathbf{P}\mathscr{H} = \{\widehat{\rho}_\psi \in L(\mathscr{H})\,|\ \widehat{\rho}_\psi = \psi\psi^\dagger \text{ for some } \psi \in S(\mathscr{H})\}\,,$$

so that elements in $\mathbf{P}\mathscr{H}$ are projection operators. The map

$$\pi : S(\mathscr{H}) \to \mathbf{P}\mathscr{H} : \psi \mapsto \psi\psi^\dagger$$

is called the ***Hopf fibration***, so that $S(\mathscr{H}) \to \mathbf{P}\mathscr{H}$ is called ***Hopf bundle***. When $\mathscr{H}$ is finite-dimensional, this map is well characterized while difficulties emerge in the infinite-dimensional case, which has been worked out in [9].

Over the years, the geometry of the projective Hilbert space has attracted much attention in quantum computation, especially in relation to holonomy [24] and Fubini-Study geodesics [2] (see Grover's algorithm [23, 33]). Even more, the emergence of the Hopf bundle stands as the origin of a continuing research on the geometric features of quantum dynamics. However, in this lecture series, we are more interested in the role of Lie group within quantum dynamics and thus we are going to start making these connections by introducing momentum maps in the context of quantum mechanics. As we shall see, the map π can be regarded as a momentum map.

2.6 Momentum maps in quantum mechanics

In geometric mechanics, momentum maps are objects taking a symplectic manifold to the dual of a Lie algebra.

Definition 2.7 (Momentum map) *Let G be a Lie group acting on a Poisson manifold $(P, \{\cdot,\cdot\})$. A momentum map is a map*

$$\mathbf{J} : P \to \mathfrak{g}^*$$

such that

$$\{F, \langle \mathbf{J}(p), \xi\rangle\} = \xi_P[F] \qquad \forall F \in C^\infty(P) \quad \forall \xi \in \mathfrak{g}\,,$$

where ξ_P denotes the infinitesimal Lie algebra action of the vector field ξ_P on the functional F.

These maps are of paramount importance, as they unfold the geometry of all the relevant objects emerging in physics, from the angular momentum to the Poynting vector in electromagnetism. In quantum mechanics (and Koopman's classical mechanics), momentum maps again explain the geometric nature of several objects in physics from the Hopf projection to expectation values.

If we were to use the geometric structure underlying the Hopf bundle, we would need to rewrite all the relations so far in terms of projections $\widehat{\rho}_\psi$. However, this becomes complicated very quickly and this is the reason why in physics one prefers to carry phases along by studying the dynamics on the Hilbert space $\mathscr{H}$. As we shall see, this does not diminish the mathematical richness of momentum map theory in quantum mechanics.

We start with an intuitive but important result:

Lemma 2.8 (Canonical representations are unitary) *Consider a symplectic Hilbert space $(\mathscr{H}, \omega)$ with symplectic form*

$$\omega(\psi_1, \psi_2) = 2\hbar\,\mathrm{Im}\langle\psi_1|\psi_2'\rangle = 2\hbar\langle i\psi_1, \psi_2\rangle$$

and consider the representation $\Phi : G \times \mathscr{H} \to \mathscr{H}$ of a Lie group G. Then, the representation is canonical if and only if it is a unitary operator on $\mathscr{H}$.

The proof is simply based on the fact that the relation

$$\omega(\Phi(g,\psi_1), \Phi(g,\psi_2)) = 2\hbar\langle i\Phi(g,\psi_1), \Phi(g,\psi_2)\rangle = 2\hbar\langle i\psi_1, \psi_2\rangle$$

holds iff Φ acts as a unitary operator. At this point, since we are on a symplectic vector space, we can define a momentum map as follows.

Definition 2.9 (Momentum map) *Let $\Phi : G \times \mathscr{H} \to \mathscr{H}$ be a unitary representation of a Lie group G (with Lie algebra $\mathfrak{g}$) on $\mathscr{H}$. A momentum map associated to Φ is a map*

$$\mathbf{J} : \mathscr{H} \to \mathfrak{g}^*$$

defined as

$$\langle \mathbf{J}(\psi), \xi\rangle = \frac{1}{2}\omega(\xi_{\mathscr{H}}(\psi), \psi) = \hbar\langle i\xi_{\mathscr{H}}(\psi), \psi\rangle \qquad\qquad \forall\psi \in \mathscr{H} \qquad \forall\xi \in \mathfrak{g}\,,$$

where $\xi_{\mathscr{H}}$ denotes the infinitesimal generator of the $G-$representation Φ.

This definition gives us a tool for computing momentum maps in an easy way. As a first step, we are interested in computing the momentum map for the standard (left) representation

$$\Phi(U, \psi) = U\psi\,, \qquad\qquad U \in \mathcal{U}(\mathscr{H})$$

of the unitary group $G = \mathcal{U}(\mathscr{H})$. We recall that the Lie algebra $\mathfrak{u}(\mathscr{H}) = T_e\mathcal{U}(\mathscr{H})$ of the unitary group $\mathcal{U}(\mathscr{H})$ is the vector space

$$\mathfrak{u}(\mathscr{H}) = \{\hat{\xi} \in L(\mathscr{H}) \,|\, \hat{\xi} = -\hat{\xi}^\dagger\}$$

of skew-Hermitian operators on $\mathscr{H}$ endowed with the commutator

$$[\hat{\xi}_1, \hat{\xi}_2] = \hat{\xi}_1\hat{\xi}_2 - \hat{\xi}_2\hat{\xi}_1\,.$$

In addition, the pairing $\langle\cdot,\cdot\rangle : \mathfrak{u}(\mathscr{H})^* \times \mathfrak{u}(\mathscr{H}) \to \mathbb{R}$ is written as

$$\langle\hat{\xi}_1, \hat{\xi}_2\rangle = \mathrm{Re}\left[\,\mathrm{Tr}(\hat{\xi}_1^\dagger\hat{\xi}_2)\right] = \mathrm{Re}\langle\hat{\xi}_1|\hat{\xi}_2\rangle\,.$$

Here, Tr denotes the ***generalized trace*** on trace-class operators[1]

$$\mathrm{Tr}(\widehat{K}) = \sum_{n=0}^{\infty}\langle w_n|\widehat{K}w_n\rangle\,,$$

[1]We notice that skew-Hermitian operators are not generally trace-class. Such obstacles emerge in infinite dimensions. Here, in order to make progress, we shall assume that all the traces considered converge appropriately. More specifically, we shall assume that expectation values exist at all times.

where $\widehat{K}$ is a bounded operator and $\{w_n\}_n$ is a basis over $\mathscr{H}$. As a last step, we notice that the infinitesimal generator of the representation $\Phi(U, \psi)$ is simply

$$\xi_{\mathscr{H}}(\psi) = \hat{\xi}\psi\,,$$

so that we are now ready to compute the momentum map:

$$\langle \mathbf{J}(\psi), \xi\rangle = \hbar\langle i\hat{\xi}\psi, \psi\rangle = \hbar\langle \psi, i\hat{\xi}\psi\rangle = \hbar\,\mathrm{Re}\left[\,\mathrm{Tr}(i\psi^\dagger\hat{\xi}\psi)\right] = \hbar\,\mathrm{Re}\left[\,\mathrm{Tr}(i\psi\psi^\dagger\hat{\xi})\right] = \langle -i\hbar\psi\psi^\dagger, \hat{\xi}\rangle$$

In conclusion, we obtain [20]

$$\mathbf{J}(\psi) = -i\hbar\psi\psi^\dagger = -i\hbar\hat{\rho}_\psi\,,$$

so that, up to a numerical factor, the momentum map equals the Hopf projection map $\pi(\psi) = \psi\psi^\dagger$. Notice that this momentum map also enjoys the equivariance property, as it is easily verified by

$$\mathbf{J}(\Phi(U, \psi)) = -i\hbar(U\psi)(U\psi)^\dagger = -i\hbar U\hat{\rho}_\psi U^{-1} = \mathrm{Ad}^*_{U^{-1}}\,\mathbf{J}(\psi)$$

and thus it is a Poisson.

The other group we have encountered is the group $\mathcal{U}(1) \simeq S^1$ of phase transformations, whose Lie algebra is easily identified with the real numbers. The phase group acts on $\mathscr{H}$ as

$$\Phi(\varphi, \psi) = e^{-i\frac{\varphi}{\hbar}}\psi$$

and the infinitesimal generator reads

$$\xi_{\mathscr{H}}(\psi) = -i\hbar\xi\psi\,.$$

Then, the momentum map is computed as

$$\langle \mathbf{J}(\psi), \xi\rangle = \hbar\langle i(-i\hbar^{-1}\xi)\psi, \psi\rangle = \xi\|\psi\|^2$$

so that the momentum map

$$\mathbf{J}(\psi) = \|\psi\|^2$$

is the total probability, which we know is preserved by the theory. We already saw how both the total energy $h(\psi) = \langle\psi|\widehat{H}\psi\rangle$ and the DF Lagrangian are both phase-invariant and thus the total probability is always conserved (by Noether's theorem) for any quantum system.

2.7 The Heisenberg group

In quantum mechanics, the Heisenberg group and its unitary representations play a fundamental role. Actually, any unitary representation of the Heisenberg group produces equivalent quantum theories [10]. In this Section, we deliberately work on the infinite-dimensional Hilbert space of square-integrable (wave)functions on $\mathbb{R}^3$.

Definition 2.10 (Heisenberg group) *Consider the symplectic vector space* $(\mathbb{R}^{2n}, \mathbb{J})$ *with the canonical symplectic form. Then, the space*

$$\mathcal{H}(\mathbb{R}^{2n}, \mathbb{J}) := \mathbb{R}^{2n} \times \mathbb{R}$$

is a Lie group endowed with the group multiplication structure

$$h_1h_2 = (\mathbf{h}_1, \varphi_1)(\mathbf{h}_2, \varphi_2) = \left(\mathbf{h}_1 + \mathbf{h}_2, \varphi_1 + \varphi_2 + \frac{1}{2}\mathbf{h}_1 \cdot \mathbb{J}\mathbf{h}_2\right),$$

where we have used the notation

$$h = (\mathbf{h}, \varphi)\,.$$

This Lie group is called the ***Heisenberg group****.*

The Lie algebra of the Heisenberg group (**Heisenberg algebra**) is given as $\mathfrak{h}(\mathbb{R}^{2n},\mathbb{J})=\mathbb{R}^{2n}\times\mathbb{R}$. Upon using the notation

$$\zeta=(\boldsymbol{\zeta},\phi)\in\mathfrak{h}(\mathbb{R}^{2n},\mathbb{J})\qquad\text{and}\qquad\mu=(\boldsymbol{\mu},\sigma)\in\mathfrak{h}(\mathbb{R}^{2n},\mathbb{J})^*\,,$$

it is easy to verify the following relations [Bonet-Luz (2016)]

$$\begin{aligned}&\mathrm{Ad}_h\,\zeta=(\boldsymbol{\zeta},\phi+\mathbf{h}\cdot\mathbb{J}\boldsymbol{\zeta})\,, &&\mathrm{Ad}^*_h\,\mu=(\boldsymbol{\mu}-\sigma\mathbb{J}\mathbf{h},\sigma)\\ &\mathrm{ad}_{\zeta_1}\,\zeta_2=(\mathbf{0},\boldsymbol{\zeta}_1\cdot\mathbb{J}\boldsymbol{\zeta}_2)\,, &&\mathrm{ad}^*_\zeta\,\mu=(-\sigma\mathbb{J}\boldsymbol{\zeta},0)\end{aligned}$$

In this Section, we aim to show how the Heisenberg group is intrinsically related to the expectation values of the canonical observables, which are written as

$$\langle\widehat{Q}\rangle=\langle\psi|\boldsymbol{x}\psi\rangle\,,\qquad\qquad\langle\widehat{P}\rangle=\langle\psi|(-i\hbar\nabla)\psi\rangle\,.$$

As we shall see, these expectation values are actually momentum maps for the Heisenberg group! In order to start our discussion, let us state the following result (see e.g. [15])

Proposition 2.11 (Heisenberg group representations) *The map*

$$\psi(\boldsymbol{x})\mapsto e^{-i\hbar^{-1}\left[\varphi+\mathbf{p}\cdot\left(\frac{\mathbf{q}}{2}-\boldsymbol{x}\right)\right]}\,\psi(\boldsymbol{x}-\mathbf{q})=:U_h\psi$$

is a (left) representation of the Heisenberg group. Upin recalling the canonical observables $\widehat{Z}=(\widehat{Q},\widehat{P})$*, the infinitesimal generator reads*

$$\xi_{\mathscr{H}}(\psi)=-i\hbar^{-1}\left(\phi\mathbf{1}+\boldsymbol{\zeta}\cdot\mathbb{J}\,\widehat{Z}\right)\psi\,,$$

Proof. Linearity is obvious. Also, it is obvious that

$$U_e=U_{(\mathbf{0},0)}\psi=\psi\,.$$

Moreover, we compute

$$\begin{aligned}(U_{h_1}U_{h_2}\psi)(\boldsymbol{x})&=U_{h_1}\left[e^{-i\hbar^{-1}\left[\varphi_2+\mathbf{p}_2\cdot\left(\frac{\mathbf{q}_2}{2}-\boldsymbol{x}\right)\right]}\,\psi(\boldsymbol{x}-\mathbf{q}_2)\right]\\ &=e^{-i\hbar^{-1}\left[\varphi_1+\mathbf{p}_1\cdot\left(\frac{\mathbf{q}_1}{2}-\boldsymbol{x}\right)\right]}\left[e^{-i\hbar^{-1}\left[\varphi_2+\mathbf{p}_2\cdot\left(\frac{\mathbf{q}_2}{2}-(\boldsymbol{x}-\mathbf{q}_1)\right)\right]}\,\psi(\boldsymbol{x}-\mathbf{q}_1-\mathbf{q}_2)\right]\\ &=e^{-i\hbar^{-1}\left[\varphi_1+\varphi_2+\mathbf{p}_2\cdot\mathbf{q}_1+\frac{1}{2}(\mathbf{q}_1\cdot\mathbf{p}_2-\mathbf{q}_2\cdot\mathbf{p}_1)-(\mathbf{p}_1+\mathbf{p}_2)\cdot\boldsymbol{x}\right]}\,\psi(\boldsymbol{x}-\mathbf{q}_1-\mathbf{q}_2)\\ &=e^{-i\hbar^{-1}\left[\varphi_1+\varphi_2+\frac{1}{2}(\mathbf{q}_1\cdot\mathbf{p}_2-\mathbf{q}_2\mathbf{p}_1)+(\mathbf{p}_1+\mathbf{p}_2)\cdot\left(\frac{\mathbf{q}_1+\mathbf{q}_2}{2}-\boldsymbol{x}\right)\right]}\,\psi(\boldsymbol{x}-\mathbf{q}_1-\mathbf{q}_2)\\ &=e^{-i\hbar^{-1}\left(\varphi_1+\varphi_2+\frac{1}{2}\mathbf{h}_1\cdot\mathbb{J}\mathbf{h}_2\right)}e^{-i\hbar^{-1}(\mathbf{p}_1+\mathbf{p}_2)\cdot\left(\frac{\mathbf{q}_1+\mathbf{q}_2}{2}-\boldsymbol{x}\right)}\,\psi(\boldsymbol{x}-(\mathbf{q}_1+\mathbf{q}_2))\\ &=(U_{h_1h_2}\psi)(\boldsymbol{x})\,.\end{aligned}$$

In addition, we apply the definition of infinitesimal generator and consider a curve $(\mathbf{h}(t),\varphi(t))\in\mathcal{H}(\mathbb{R}^{2n})$ such that

$$(\mathbf{h}(0),\varphi(0))=(\mathbf{q}(0),\mathbf{p}(0),\varphi(0))=0\qquad\text{and}\qquad(\dot{\mathbf{h}}(0),\dot\varphi(0))=(\boldsymbol{\zeta},\phi)=(\boldsymbol{q},\boldsymbol{p},0)\in\mathfrak{h}(\mathbb{R}^{2n})$$

and compute

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\Big|_0 \left[e^{-i\hbar^{-1}\left[\varphi(t)+\mathbf{p}(t)\cdot\left(\frac{\mathbf{q}(t)}{2}-\boldsymbol{x}\right)\right]}\,\psi(\boldsymbol{x}-\mathbf{q}(t))\right] \\
&= e^{-i\hbar^{-1}\left[\varphi+\mathbf{p}\cdot\left(\frac{\mathbf{q}}{2}-\boldsymbol{x}\right)\right]}\left\{-i\kappa\left[\dot\varphi+\dot{\mathbf{p}}\cdot\left(\frac{\mathbf{q}}{2}-\boldsymbol{x}\right)+\frac{\mathbf{p}\cdot\dot{\mathbf{q}}}{2}\right]\psi(\boldsymbol{x}-\mathbf{q})-\dot{\mathbf{q}}\cdot\nabla\psi(\boldsymbol{x}-\mathbf{q})\right\}\Big|_0 \\
&= \;-i\hbar^{-1}\left(\phi-\boldsymbol{p}\cdot\boldsymbol{x}\right)\psi(\boldsymbol{x})-\boldsymbol{q}\cdot\nabla\psi(\boldsymbol{x}) \\
&= \;-i\hbar^{-1}\left(\phi\mathbf{1}-\boldsymbol{p}\cdot\boldsymbol{x}\right)\psi(\boldsymbol{x})-i\hbar^{-1}\boldsymbol{q}\cdot(-i\hbar\nabla)\psi(\boldsymbol{x}) \\
&= \;-i\hbar^{-1}\big(\phi\mathbf{1}-\boldsymbol{p}\cdot\boldsymbol{x}+\boldsymbol{q}\cdot(-i\hbar\nabla)\big)\psi(\boldsymbol{x}) \\
&= \;-i\hbar^{-1}\left[\phi\mathbf{1}+\boldsymbol{\zeta}\cdot\mathbb{J}\widehat{Z}\right]\psi(\mathbf{z})\,.
\end{aligned}
$$

Here, we have recalled the standard definition (5) of the canonical observables. ■

2.8 Expectation values as momentum maps

At this point, in order to proceed to momentum maps, it is convenient to recall the following Lemma:

Lemma 2.12 *With the notation above, we have*

$$U_h\widehat{Z}U_h^{-1}=\widehat{Z}-\mathbf{h}\mathbf{1}\,.$$

Proof. Here we use the notation $\mathbf{h}=(\mathbf{h}_q,\mathbf{h}_p)$. The first relation is easily proved by a direct verification. The first component reads as follows:

$$
\begin{aligned}
\big(U_h\widehat{Q}U_h^\dagger\big)\psi(\boldsymbol{x}) &= \big(U_h\boldsymbol{x}\big)\left[e^{\frac{i}{\hbar}\varphi}e^{-i\frac{\mathbf{h}_p\cdot\mathbf{h}_q}{2\hbar}}e^{-i\frac{\mathbf{h}_p\cdot\boldsymbol{x}}{\hbar}}\psi(\boldsymbol{x}+\mathbf{h}_q)\right] \\
&= e^{-i\frac{\mathbf{h}_p\cdot\mathbf{h}_q}{\hbar}}e^{i\frac{\mathbf{h}_p\cdot\boldsymbol{x}}{\hbar}}(\boldsymbol{x}-\mathbf{h}_q)e^{-i\frac{\mathbf{h}_p\cdot(\boldsymbol{x}-\mathbf{h}_q)}{\hbar}}\psi(\boldsymbol{x}) \\
&= (\boldsymbol{x}-\mathbf{h}_q)\psi(\boldsymbol{x})\,.
\end{aligned}
$$

Similarly, the second component reads

$$
\begin{aligned}
\big(U_h\widehat{P}U_h^\dagger\big)\psi(\boldsymbol{x}) &= -i\hbar\left(U_h\nabla\right)\left[e^{\frac{i}{\hbar}\varphi}e^{-i\frac{\mathbf{h}_p\cdot\mathbf{h}_q}{2\hbar}}e^{-i\frac{\mathbf{h}_p\cdot\boldsymbol{x}}{\hbar}}\psi(\boldsymbol{x}+\mathbf{h}_q)\right] \\
&= -U_h\left[e^{\frac{i}{\hbar}\varphi}e^{-i\frac{\mathbf{h}_p\cdot\mathbf{h}_q}{2\hbar}}e^{-i\frac{\mathbf{h}_p\cdot\boldsymbol{x}}{\hbar}}\big(\mathbf{h}_p\,\psi(\boldsymbol{x}+\mathbf{h}_q)+i\hbar\nabla\psi(\boldsymbol{x}+\mathbf{h}_q)\big)\right] \\
&= (-\mathbf{h}_p+P)\psi(\boldsymbol{x})\,.
\end{aligned}
$$

Then, the proof is complete. ■

We are now ready to show how expectation values are actually momentum maps:

Proposition 2.13 [5] *The momentum map associated to the previous unitary representation reads*

$$J(\psi)=\left(\mathbb{J}\langle\widehat{Z}\rangle,\|\psi\|^2\right)\,.$$

Also, this momentum map is equivariant.

Proof. The momentum map property follows as a direct verification:

$$\langle J(\psi),\zeta\rangle=\frac{1}{2}\,\omega(\zeta_{\mathscr{H}}[\psi],\psi)=\langle(\phi+\boldsymbol{\zeta}\cdot\mathbb{J}\widehat{Z})\psi|\psi\rangle=\phi\|\psi\|^2+\boldsymbol{\zeta}\cdot\mathbb{J}\langle\widehat{Z}\rangle=\Big\langle(\mathbb{J}\langle\widehat{Z}\rangle,\|\psi\|^2),\,(\boldsymbol{\zeta},\phi)\Big\rangle\,,$$

where we denoted $\xi=(\boldsymbol{\zeta},\phi)$.

Equivariance follows by using the previous Lemma. We compute

$$\mathbf{J}(U_h\psi)=(\mathbb{J}\langle U_h^{-1}\widehat{Z}U_h\rangle,\|\psi\|^2\rangle)=(\|\psi^2\|\mathbb{J}\mathbf{h}+\mathbb{J}\langle\widehat{Z}\rangle,\,\|\psi\|^2\rangle)=\mathrm{Ad}^*_{h^{-1}}\,\mathbf{J}(\psi)\,,$$

so that the proof is complete. ■

An interesting consequence of this result is that the canonical Poisson bracket of classical mechanics is actually recovered naturally by simply recalling the Lie-Poisson reduction theorem [Marsden & Ratiu (1998)]. Indeed, since equivariant momentum map are also Poisson, we have

$$\{F\circ\mathbf{J},K\circ\mathbf{J}\}_{\mathscr{H}}=\{F,K\}_{\mathfrak{h}^*}\circ\mathbf{J}\,,\qquad\forall F,K\in C^\infty(\mathfrak{h}^*)\,,$$

where we have used the short hand notation $\mathfrak{h}^*=\mathfrak{h}(\mathbb{R}^{2n})$ and $\{F,K\}_{\mathfrak{h}^*}$ denotes the (+)Lie-Poisson bracket on $\mathfrak{h}^*$. The latter reads explicitly as

$$\{F,K\}_{\mathfrak{h}^*}(\boldsymbol{\mu},\sigma)=\sigma\,\frac{\partial F}{\partial\boldsymbol{\mu}}\cdot\mathbb{J}\frac{\partial K}{\partial\boldsymbol{\mu}}\,.$$

Then, if we now denote

$$(\boldsymbol{\mu},\sigma)=\mathbf{J}(\psi)=(\mathbb{J}\langle\widehat{Z}\rangle,\|\psi\|^2)=:(\mathbb{J}\boldsymbol{z},\sigma)\,,$$

a change of variables yields

$$\{F,K\}_{\mathfrak{h}^*}(\boldsymbol{z},\sigma)=\sigma\,\frac{\partial F}{\partial\boldsymbol{z}}\cdot\mathbb{J}\frac{\partial K}{\partial\boldsymbol{z}}\,,$$

so that the normalization condition $\sigma=\|\psi\|^2=1$ returns the canonical Poisson bracket.

It may seem surprising that momentum maps for the Heisenberg group representation takes us back from quantum to classical mechanics. This is a specific feature of the Heisenberg group, which generates a specific class of states which obey an equivalent form of classical motion. Interestingly enough, the momentum map structure of expectation values has never appeared before in the literature and it was first presented only recently in [5].

2.9 Coherent states as group orbits

Among all possible wavefunctions, there is a very special class that has attracted much attention over the decades, especially because of their geometric properties, which confer them several analogies with classical trajectories. While different definitions of quantum states are available, here we shall use the one that is due to [25]. According to Perelomov's definition, coherent states are ***orbits of the Heisenberg group***. We recall that the orbit of an element $\psi_0\in\mathscr{H}=L^2(\mathbb{R}^3)$ is given as

$$\mathrm{Orb}(\psi_0)=\{U_h\psi_0\,|\,h\in\mathcal{H}(\mathbb{R}^{2n},\mathbb{J})\}\,.$$

Perelomov's result can be stated as follows:

Definition 2.14 (Perelomov (1971)) *Let* $\psi \in \mathscr{H} = L^2(\mathbb{R}^3)$*. Then,* ψ *is a coherent state if and only if there exists* $\psi_0 \in \mathscr{H}$ *such that*

$$\psi \in \mathrm{Orb}(\psi_0)\,.$$

We are interested in writing the Schrödinger equation whose solution is always a coherent state. This can be easily found by taking the time derivative of the relation

$$\psi(t) = U_{h(t)}\psi_0\,.$$

This gives

$$\dot{\psi} = \dot{U}_h U_h^{-1}\psi = \xi_{\mathscr{H}}(\psi) = -i\hbar^{-1}(\phi\mathbf{1} + \boldsymbol{\zeta}\cdot\mathbb{J}\widehat{Z})\psi$$

or, by dropping the phase term $\phi\psi$ and recalling the notation $\boldsymbol{\zeta} = (\boldsymbol{q}, \boldsymbol{p})$,

$$i\hbar\dot{\psi}(\boldsymbol{x}) = \boldsymbol{q}\cdot\boldsymbol{x}\psi(\boldsymbol{x}) + i\hbar\boldsymbol{p}\cdot\nabla\psi(\boldsymbol{x}) =: \widehat{H}\psi(\boldsymbol{x})\,.$$

The conclusion is that the Schrödinger equation associated to Hamiltonian operators that are linear in the canonical observables are coherent states, whose expectation values evolve according to Ehrenfest's relations (3), that is by translations in phase-space:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\widehat{Z}\rangle = i\hbar^{-1}\langle[\boldsymbol{\zeta}\cdot\mathbb{J}\widehat{Z}, \widehat{Z}]\rangle = \boldsymbol{\zeta}\,.$$

Here he have used the canonical commutation relations (4) in the form

$$[\widehat{Z}^h, \widehat{Z}^k] = i\hbar\mathbb{J}^{hk}\,.$$

In practical applications, one considers the specific case where

$$\psi_0(\boldsymbol{x}) = \frac{1}{(\pi\hbar)^{1/4}}\, e^{\frac{-|\boldsymbol{x}|^2}{2\hbar}}\,,$$

which appears in practical applications as one of the solutions of the Schrödinger equation associated to the Hamiltonian operator $\widehat{H} = \widehat{P}^2/2 + \widehat{Q}/2$ (quantum harmonic oscillator). This particular choice has the special feature of minimizing uncertainty, that is

$$\sqrt{\langle(\widehat{Q} - \langle\widehat{Q}\rangle)^2\rangle}\sqrt{\langle(\widehat{P} - \langle\widehat{P}\rangle)^2\rangle} = \frac{\hbar}{2}\,,$$

where all expectation values are computes with respect to ψ_0. In chemical physics, the wavefunction of a coherent state $\psi(t) = U_{h(t)}\psi_0$ is called *frozen Gaussian wavepacket* [16].

The characterization of coherent states in terms of orbits associated to unitary representation allowed Perelomov to generalize this construction to arbitrary group representations. For example, in the finite dimensional case when $\mathscr{H} = \mathbb{C}^2$, the standard representation of $SU(2)$ yields the *spin coherent states*. The classification of coherent states for different unitary representations is an entire chapter of mathematical physics on its own right.

3 Euler-Poincaré theory of quantum dynamics

3.1 The Euler-Poincaré theorem

In this lecture series, we assume previous knowledge of Euler-Poincaré reduction. Thus, we are only going to state the theorem without going into the details and its proof. Here, the original theorem [17] is slightly extended by following [14].

Theorem 3.1 (Euler-Poincaré reduction) *Consider the following hypohteses.*

- *Consider a Lie group G and a left action on a manifold M. For a given $a_0 \in M$, let*

$$L_{a_0} : TG \to \mathbb{R}$$

be a Lagrangian with symmetry-breaking parameter a_0.

- *Then, define the unique function (if it exists)*

$$\begin{aligned} &L : TG \times M \to \mathbb{R} \\ &L(g, \dot{g}, a_0) := L_{a_0}(g, \dot{g}) \quad \forall (g, \dot{g}) \in TG. \end{aligned}$$

such that L is invariant under the left action

$$\begin{aligned} &G \times (TG \times M) \to TG \times M \\ &\big(h, (g, \dot{g}, a_0)\big) \mapsto (hg, h\dot{g}, ha_0). \end{aligned}$$

- *Also, define*

$$L\left(g^{-1}g,\ g^{-1}\dot{g},\ g^{-1}a_0\right) =: \ell(\xi, a),$$

where

$$a := g^{-1}a_0, \qquad \xi := g^{-1}\dot{g}.$$

Then, the following are equivalent:

1. *Hamilton's principle*

$$\delta \int_{t_1}^{t_2} L_{a_0}(g, \dot{g})\, dt = 0$$

holds for $\delta g(t_1) = \delta g(t_2) = 0$.

2. *$g(t)$ satisfies the Euler-Lagrange equations.*

3. *The reduced Hamilton's principle*

$$\delta \int_{t_1}^{t_2} \ell(\xi, a)\, dt = 0$$

holds on $\mathfrak{g} \times M$, using variations

$$\delta\xi = \dot{\eta} + ad_\xi \eta, \qquad \delta a = -\eta_M(a),$$

with $\eta(t_1) = \eta(t_2) = 0$.

4. *The Euler-Poincaré equations*

$$\frac{d}{dt}\frac{\partial \ell}{\partial \xi} = \operatorname{ad}^*_\xi \frac{\partial \ell}{\partial \xi} - a \diamond \frac{\partial \ell}{\partial a} \qquad \dot{a} = -\xi_M a$$

hold on $\mathfrak{g} \times M$*, where*

$$\left\langle \frac{\partial \ell}{\partial a}\,,\, \zeta_M a \right\rangle =: \left\langle a \,\diamond\, \frac{\partial \ell}{\partial a}\,,\, \zeta \right\rangle \qquad \forall \zeta \in \mathfrak{g}\,,\; \forall a \in M.$$

Remark (Pairing notations). Notice that the above definition of the diamond operator involves two different pairings. Indeed, while the left hand side involves the pairing between cotangent and tangent vectors on the manifold M (i.e. $\langle \cdot\,, \cdot\rangle : T^*_a M \times T_a M \to \mathbb{R}$), the right hand side involves the pairing between vectors and covectors on the Lie algebra $\mathfrak{g}$ (i.e. $\langle \cdot\,, \cdot\rangle : \mathfrak{g}^* \times \mathfrak{g} \to \mathbb{R}$). Although one might think of using different notations for the two pairings, no confusion should arise when using the same notation as above.

3.2 Euler-Poincaré formulation for pure quantum states

This section presents the Euler-Poincaré formulation of quantum dynamics in the Schrödinger picture [4]. The main example we consider is the quantum dynamics as it arises from the Dirac-Frenkel Lagrangian. The results in this Section are obtained by proceeding formally and the infinite-dimensional case $\mathscr{H} = L^2(\mathbb{R}^3)$ may need extra care when dealing convergence issues. Here, we shall ignore this type of problems and assume that the wavefunctions behave in such a way that expectation values always converge.

Upon denoting by $T\mathscr{H}$ the tangent bundle of the Hilbert space $\mathscr{H}$, consider a generic Lagrangian

$$L : T\mathscr{H} \to \mathbb{R}\,, \qquad L = L(\psi, \dot{\psi})\,, \tag{9}$$

so that the assumption of quantum evolution restricts ψ to evolve under the action of that unitary group $\mathcal{U}(\mathscr{H})$, that is

$$\psi(t) = U(t)\psi_0\,, \qquad U(t) \in \mathcal{U}(\mathscr{H}) \tag{10}$$

where ψ_0 is some initial condition, whose normalization is ordinarily chosen such that $\|\psi_0\|^2 = 1$. Then, $\psi_0 \in S(\mathscr{H})$ implies $\psi(t) \in S(\mathscr{H})$ at all times.

The relation (10) takes the Lagrangian $L(\psi, \dot{\psi})$ to a Lagrangian of the type $L_{\psi_0}(U, \dot{U})$, which then produces Euler-Lagrange equations for the Lagrangian coordinate $U \in \mathcal{U}(\mathscr{H})$. Moreover, by following Euler-Poincaré theory, one denotes by $\mathfrak{u}(\mathscr{H})$ the Lie algebra of skew Hermitian operators and defines

$$\xi(t) := \dot{U}(t)U^{-1}(t) \in \mathfrak{u}(\mathscr{H})\,.$$

Since $\dot{\psi} = \xi\psi$, one obtains the reduced Lagrangian

$$\ell : \mathfrak{u}(\mathscr{H}) \times \mathscr{H} \to \mathbb{R}\,, \qquad \ell(\xi, \psi) := L(\psi, \xi\psi)$$

and the Euler-Poincaré variational principle

$$\delta\int_{t_1}^{t_2}\ell(\xi,\psi)\,\mathrm{d}t=0\,. \tag{11}$$

Then, upon computing

$$\delta\xi=\dot\eta+[\eta,\xi]\,,\qquad \delta\psi=\eta\psi \tag{12}$$

where $\eta:=(\delta U)U^{-1}$, one obtains the following result.

Theorem 3.2 *Consider the variational principle (11) with the auxiliary equation $\dot\psi=\xi\psi$ and the variations (12), where η is arbitrary and vanishes at the endpoints. This variational principle is equivalent to the equations of motion*

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta\ell}{\delta\xi}-\left[\xi,\frac{\delta\ell}{\delta\xi}\right]=\frac{1}{2}\left(\frac{\delta\ell}{\delta\psi}\psi^\dagger-\psi\frac{\delta\ell}{\delta\psi}^\dagger\right),\qquad\qquad \frac{\mathrm{d}\psi}{\mathrm{d}t}=\xi\psi\,. \tag{13}$$

Proof. The proof is a direct verification. We compute

$$\begin{aligned}\delta\int_{t_0}^{t_1}\ell(\xi,\psi)\,\mathrm{d}t&=\int_{t_0}^{t_1}\left(\left\langle\frac{\delta\ell}{\delta\xi},\delta\xi\right\rangle+\left\langle\frac{\delta\ell}{\delta\psi},\delta\psi\right\rangle\right)\,\mathrm{d}t\\&=\int_{t_0}^{t_1}\left(\left\langle\frac{\delta\ell}{\delta\xi},\dot\eta+[\eta,\xi]\right\rangle+\left\langle\frac{\delta\ell}{\delta\psi},\eta\psi\right\rangle\right)\,\mathrm{d}t\\&=\int_{t_0}^{t_1}\left(\left\langle-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta\ell}{\delta\xi}+\left[\xi,\frac{\delta\ell}{\delta\xi}\right],\eta\right\rangle+\left\langle\frac{\delta\ell}{\delta\psi}\psi^\dagger,\eta\right\rangle\right)\,\mathrm{d}t\\&=\int_{t_0}^{t_1}\left[\left\langle-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta\ell}{\delta\xi}+\left[\xi,\frac{\delta\ell}{\delta\xi}\right],\eta\right\rangle+\frac{1}{2}\left\langle\left(\frac{\delta\ell}{\delta\psi}\psi^\dagger-\psi\frac{\delta\ell}{\delta\psi}^\dagger\right),\eta\right\rangle\right]\,\mathrm{d}t\,,\end{aligned}$$

where last equality follows from the fact that η is skew-Hermitian. Then, the first equation in (13) follows since η is arbitrary. ■

Here, we use the ordinary definition of variational derivative

$$\delta F(q):=\left\langle\frac{\delta F}{\delta q},\delta q\right\rangle,$$

for any function(al) $F\in C^\infty(M)$ on the manifold M. In typical situations, the reduced Lagrangian is quadratic in ψ, so that the $\mathcal{U}(1)$-invariance under phase transformations takes the dynamics to the projective space $\mathbf{P}\mathscr{H}$. Indeed, as we shall see, the reduced Lagrangian $\ell(\xi,\psi)$ can be written typically in terms of the projection $\rho_\psi=\psi\psi^\dagger$ to produce a new Lagrangian

$$l:\mathfrak{u}(\mathscr{H})\times\mathbf{P}\mathscr{H}\to\mathbb{R}\,,\qquad l(\xi,\rho_\psi)=\ell(\xi,\psi)\,.$$

In this case, a direct calculation using $\rho_\psi=U\psi_0\psi_0^\dagger U^\dagger$ shows that

$$\delta\rho_\psi=[\eta,\rho_\psi]\,,\qquad \dot\rho_\psi=[\xi,\rho_\psi] \tag{14}$$

and the previous theorem specializes as follows (the proof is omitted here, as it proceeds in exactly the same was as in the previous case)

Theorem 3.3 *Consider the variational principle $\delta\int_{t_1}^{t_2} l(\xi,\rho_\psi)\,\mathrm{d}t = 0$ with the relations (14) and $\delta\xi = \dot\eta + [\eta,\xi]$, where η is arbitrary and vanishes at the endpoints. This variational principle is equivalent to the equations of motion*

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta l}{\delta\xi} - \left[\xi, \frac{\delta l}{\delta\xi}\right] = \left[\frac{\delta l}{\delta\rho_\psi}, \rho_\psi\right], \qquad \dot\rho_\psi = [\xi,\rho_\psi]\,. \tag{15}$$

Then, the unitary symmetry properties of the Lagrangian naturally take the evolution to the correct quantum state space (for pure states), that is the projective space $\mathbf{P}\mathscr{H}$. In the following sections, we shall specialize this construction to two particular examples and we shall present the momentum map properties of the underlying geometry as well as their relation to the usual principal connections appearing in the literature.

3.2.1 Euler-Poincaré dynamics on the sphere

It is easy to see that upon following the construction from the previous section, the DF Lagrangian

$$L(\psi,\dot\psi) = \left\langle \psi, i\hbar\dot\psi - H\psi\right\rangle \tag{16}$$

produces the Euler-Poincaré variational principle

$$\delta\int_{t_1}^{t_2}\langle\psi, i\hbar\xi\psi - H\psi\rangle\,\mathrm{d}t = 0$$

For simplicity, here we are considering a time-independent Hamiltonian operator H. Then, upon computing

$$\frac{\delta l}{\delta\psi} = 2(i\hbar\xi - H)\psi, \qquad \frac{\delta l}{\delta\xi} = -i\hbar\psi\psi^\dagger\,,$$

the first of (13) yields

$$[(i\hbar\xi - H)\,,\psi\psi^\dagger] = 0\,, \qquad \text{with} \qquad \dot\psi = \xi\psi\,. \tag{17}$$

Now, if we apply the first equation to ψ, we have

$$(i\hbar\xi - H)\psi = \langle\psi|(i\hbar\xi - H)\psi\rangle\psi$$

or, equivalently,

$$(\mathbf{1} - \psi\psi^\dagger)(i\hbar\xi - H)\psi = 0\,,$$

thereby returning the Schrödinger equation on the sphere (8). Somehow, the Euler-Poincaré construction has taken care of the geometry for us by returning the dynamics on the correct space, which is $S(\mathscr{H})$.

How is it possible that we started from a Lagrangian (DF) that gives us the Schrödinger equation on the Hilbert space and we end up with another Lagrangian (EP) that returns the Schrödinger equation on the sphere? The answer lies in the evolution ansatz

$$\psi(t) = U(t)\psi_0\,.$$

Indeed, the action of the unitary group on the whole Hilbert space $\mathscr{H}$ is not transitive. We recall the a $G-$action on M is transitive iff

$$\forall x,y\in M \qquad \exists g\in G \quad \text{such that} \quad gx = y\,.$$

In practice, an action is transitive if we can reach every element in M by acting on a fixed point $x_0 \in M$ with some group element $g \in G$. Now, this is not the case, for example, for $SO(3)$ acting on $\mathbb{R}^3$ and it is not the case of $\mathcal{U}(\mathscr{H})$ acting on $\mathscr{H}$. However, both these actions are indeed transitive when we restrict to consider the spheres S^2 and $S(\mathscr{H})$, respectively. Thus, it is no surprise that we do not recover the Schrödinger equation on the whole Hilbert space: we are not reaching all possible vectors in $\mathscr{H}$ with our action!

3.2.2 Euler-Poincaré dynamics on the projective Hilbert space

The situation becomes more natural if we consider the dynamics on the projective Hilbert space. It is easy to see that upon following the previous construction, the DF Lagrangian (16) produces the action functional

$$\int_{t_1}^{t_2} \Big\langle U\psi_0, i\hbar\dot{U}\psi_0 - HU\psi_0 \Big\rangle \, \mathrm{d}t = \int_{t_1}^{t_2} \Big\langle U\psi_0\psi_0^\dagger, i\hbar\dot{U} - HU \Big\rangle \, \mathrm{d}t \, .$$

Then, we can consider the Lagrangian

$$L_{\rho_0}(U, \dot{U}) = \Big\langle U\psi_0\psi_0^\dagger, i\hbar\dot{U} - HU \Big\rangle \, ,$$

where we have denoted

$$\rho_0 = \psi_0\psi_0^\dagger \in \mathbf{P}\mathscr{H} \, .$$

Then, since

$$U\psi_0\psi_0^\dagger = \psi\psi^\dagger U^\dagger = \rho_\psi U^\dagger \, ,$$

we obtains the reduced Euler-Poincaré Lagrangian

$$l : \mathfrak{u}(\mathscr{H}) \times \mathbf{P}\mathscr{H} \to \mathbb{R} \, , \qquad l(\xi, \rho_\psi) = \langle\langle \rho_\psi, i\hbar\xi - H \rangle\rangle \, .$$

We notice that now we are exploiting the $\mathcal{U}(\mathscr{H})-$action on $\mathbf{P}\mathscr{H}$, which is actually transitive (indeed, $\mathbf{P}\mathscr{H}$ is a quotient space of the sphere $S(\mathscr{H})$, where the action was already transitive) and thus we shall be able to write an equation of motion on $\mathbf{P}\mathscr{H}$.

For simplicity, here we are considering a time-independent Hamiltonian operator H. Then, upon computing

$$\frac{\delta l}{\delta \rho_\psi} = 2(i\hbar\xi - H), \qquad \frac{\delta l}{\delta \xi} = -i\hbar\rho_\psi \, ,$$

the first of (13) yields

$$[(i\hbar\xi - H) \, , \rho_\psi] = 0 \, , \qquad \text{with} \qquad \dot{\rho}_\psi = [\xi, \rho_\psi] \, . \tag{18}$$

Then, the above equations combine into the ***quantum Liouville equation for pure state dynamics***

$$i\hbar\dot{\rho}_\psi = [H, \rho_\psi]$$

This equation is also known as *Liouville-von Neuman equation* and is widely used in quantum mechanics.

4 Mixing classical and quantum

4.1 The Ehrenfest mean-field model

In chemical physics, one is interested in performing molecular dynamics simulations for systems of several particles. In typical situations, the number of particles makes the problem intractable with full quantum simulations and one wants to treat a part of the particles classically and the other part with a quantum approach.

For our purposes, here we shall consider two particles so that the wavefunction is written as

$$\Psi = \Psi(\boldsymbol{x}, \boldsymbol{r}) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)\,.$$

Also, we shall neglect other effects arising from possible extra degrees of freedom such as spin (not covered in these notes). We think of the coordinate $\boldsymbol{x}$ as that corresponding to the quantum particle, while $\boldsymbol{r}$ corresponds to the particle that we will aim to treat classically. The classical limit of quantum mechanics is subject of a continuing debate and we shall not dwell upon such topics. For our purposes, we follow an approach based on coherent states and expectation values that goes back to Ehrenfest. The variational approach presented here slightly generalizes the one presented in [Bonet-Luz (2015)].

In physics, a mean-field ansatz is of the type

$$\Psi(\boldsymbol{x}, \boldsymbol{r}, t) = \psi(\boldsymbol{x}, t)\chi(\boldsymbol{r}, t)\,,$$

where $\chi(\boldsymbol{r})$ is thought of as the wavefunction corresponding to the particle we want to treat classically. We notice that the Hamiltonian operator is now of the type

$$\widehat{H} = \widehat{H}(\widehat{Z}, \widehat{\Gamma})\,,$$

where $\widehat{\Gamma} = (\boldsymbol{r}, -i\hbar\nabla_{\boldsymbol{r}})$.

At this level, there is no assumption that relates anything to classical features. However, now we shall assume that χ is a coherent state so that

$$\chi(t) = U_{h(t)}\chi_0\,, \qquad\qquad h(t) = (\mathbf{h}(t), \varphi(t))$$

and we replace this ansatz in the DF Lagrangian. Upon recalling the pairing

$$\langle \Psi_1, \Psi_2 \rangle = \operatorname{Re} \int_{\mathbb{R}^6} \Psi_1^*(\boldsymbol{x}, \boldsymbol{r})\Psi_2(\boldsymbol{x}, \boldsymbol{r})\, \mathrm{d}^3x\, \mathrm{d}^3r$$

which becomes

$$\begin{aligned} L(\Psi, \dot{\Psi}) = &\ \left\langle \psi\chi, i\hbar\dot{\psi}\chi + i\hbar\psi\dot{\chi} \right\rangle - \left\langle \psi\chi, \widehat{H}\psi\chi \right\rangle \\ &= \langle \psi, i\hbar\dot{\psi} \rangle + \langle \chi, i\hbar\dot{\chi} \rangle - \langle \psi\,, H'\psi \rangle \\ &= \langle \psi, i\hbar\dot{\psi} \rangle + \langle \chi_0, i\hbar\dot{U}_h\chi_0 \rangle - \langle \psi\,, H'\psi \rangle =: L'(\psi, \dot{\psi}, h, \dot{h})\,, \end{aligned}$$

where we have introduced

$$H' = \int_{\mathbb{R}^3} \chi^*(\boldsymbol{r}, t)\widehat{H}\chi(\boldsymbol{r}, t)\, \mathrm{d}^3r = \int_{\mathbb{R}^3} \chi_0^*(\boldsymbol{r})U_h^{-1}\widehat{H}U_h\chi_0(\boldsymbol{r})\, \mathrm{d}^3r = H'(\mathbf{h})\,.$$

This is a Hermitian operator that depend parametrically on $\mathbf{h}(t)$, while it does not depend on the phase factor $\varphi(t)$. Notice that we have obtained a Lagrangian, which is defined as a map

$$L' : T\mathscr{H} \times T\mathcal{H} \to \mathbb{R}\,,$$

where $\mathscr{H} = L^2(\mathbb{R}^3)$ and $\mathcal{H}$ is shorthand for $\mathcal{H}(\mathbb{R}^{2n}, \mathbb{J})$, that is the Heisenberg group. At this point, one writes

$$\dot{U}_h\chi_0 = \dot{U}_h U_h^{-1}\chi = \xi_{\mathscr{H}}(\chi) = -i\hbar^{-1}(\phi + \boldsymbol{\zeta}\cdot\mathbb{J}\widehat{\Gamma})\chi$$

so that

$$\langle\chi_0, i\hbar\dot{U}_h\chi_0\rangle = \langle\chi, (\phi + \boldsymbol{\zeta}\cdot\mathbb{J}\widehat{\Gamma})\chi\rangle = \phi\|\chi\|^2 + \boldsymbol{\zeta}\cdot\mathbb{J}\langle\chi, \widehat{\Gamma}\chi\rangle\,.$$

In addition, upon recalling $\|\chi_0\|^2 = \|\chi\|^2 = 1$ as well as the notation $h = (\mathbf{h}, \varphi) \in \mathcal{H}(\mathbb{R}^{2n}, \mathbb{J})$, we observe that

$$\langle\chi, \widehat{\Gamma}\chi\rangle = \langle\chi_0, U_h^{-1}\widehat{\Gamma}U_h\chi_0\rangle = \langle\chi_0, (\widehat{\Gamma} + \mathbf{h}\mathbf{1})\chi_0\rangle = \langle\chi_0, \widehat{\Gamma}\chi_0\rangle + \|\chi\|^2\mathbf{h} =: \mathbf{z}_0 + \mathbf{h} =: \mathbf{z}$$

and, upon defining $\widetilde{H}(\mathbf{z}) = H'(\mathbf{h}) = H'(\mathbf{z} - \mathbf{z}_0)$, the Lagrangian becomes

$$L'(\psi, \dot{\psi}, \zeta, \mathbf{z}) = \phi + \boldsymbol{\zeta}\cdot\mathbb{J}\mathbf{z} + \langle\psi, i\hbar\dot{\psi}\rangle - \langle\psi\,, \widetilde{H}(\mathbf{z})\psi\rangle$$

At this point, letting $\psi = U\psi_0$ yields the Euler-Poincaré Lagrangian

$$\ell(\xi, \rho_\psi, \zeta, \mathbf{z}) = \phi + \boldsymbol{\zeta}\cdot\mathbb{J}\mathbf{z} + \langle\rho_\psi, i\hbar\xi\rangle - \langle\rho_\psi\,, \widetilde{H}(\mathbf{z})\rangle\,. \tag{19}$$

Now, this Lagrangian is defined as a map

$$\ell : \big(\mathfrak{h}(\mathbb{R}^{2n}, \mathbb{J}) \oplus \mathfrak{u}(\mathscr{H})\big) \times (\mathbb{R}^{2n} \times \mathbf{P}\mathscr{H}) \to \mathbb{R}$$

which is an Euler-Poincaré Lagrangian of the type $l : \mathfrak{g} \times M$ with $\mathfrak{g} = \mathfrak{h}(\mathbb{R}^{2n}, \mathbb{J}) \oplus \mathfrak{u}(\mathscr{H})$ and $M = \mathbb{R}^{2n} \times \mathbf{P}\mathscr{H}$. Here, the action of $\mathcal{H}(\mathbb{R}^{2n}, \mathbb{J})$ on $\mathbb{R}^{2n}$ is simply given by translations

$$h : \mathbf{z}_0 \mapsto \mathbf{z}_0 + \mathbf{h}$$

so that the infinitesimal generator is simply

$$\xi_{\mathbb{R}^{2n}}(\mathbf{z}) = \boldsymbol{\zeta}\,,$$

where we recall the notation $\xi = (\boldsymbol{\zeta}, \phi) \in \mathfrak{h}(\mathbb{R}^{2n}, \mathbb{J})$.

Theorem 4.1 *Consider the variational principle*

$$\delta\int_{t_1}^{t_2}\Big(\phi + \boldsymbol{\zeta}\cdot\mathbb{J}\mathbf{z} + \big\langle\rho_\psi, i\hbar\xi - \widetilde{H}(\mathbf{z})\big\rangle\Big)\,\mathrm{d}t = 0 \tag{20}$$

and the variations

$$(\delta\boldsymbol{\zeta}, \delta\phi) = \big(\dot{\boldsymbol{\gamma}},\, \dot{\theta} + \boldsymbol{\zeta}\cdot\mathbb{J}\boldsymbol{\gamma}\big)\,, \qquad \delta\xi = \dot{\eta} - [\xi, \eta]\,, \qquad \delta\mathbf{z} = \boldsymbol{\gamma}\,, \qquad \delta\rho_\psi = [\eta, \rho_\psi]\,,$$

where $(\boldsymbol{\gamma}, \theta)$ and η are arbitrary and vanish at the endpoints. Together with the auxiliary equations

$$\dot{\mathbf{z}} = \boldsymbol{\zeta}\,, \qquad \dot{\rho}_\psi = [\xi, \rho_\psi]\,,$$

this variational principle is equivalent to the ***Ehrenfest mean-field equations***

$$\dot{\mathbf{z}} = \mathbb{J}\nabla_{\mathbf{z}}\langle\rho_\psi|\widetilde{H}(\mathbf{z})\rangle\,, \qquad i\hbar\dot{\rho_\psi} = \Big[\widetilde{H}(\mathbf{z}), \rho_\psi\Big]\,.$$

Proof. Consider the general Lagrangian of the form $\ell(\boldsymbol{\zeta},\phi,\xi,\mathbf{z},\rho_\psi)$. By direct substitution of the variations into the variational principle

$$\delta\int_{t_1}^{t_2}\bigg(\Big\langle\frac{\delta\ell}{\delta\boldsymbol{\zeta}},\,\dot{\boldsymbol{\gamma}}\Big\rangle+\Big\langle\frac{\delta\ell}{\delta\phi},\,\dot\theta+\boldsymbol{\zeta}\cdot\mathbb{J}\boldsymbol{\gamma}\Big\rangle+\Big\langle\frac{\delta\ell}{\delta\xi},\,\dot\eta-[\xi,\eta]\Big\rangle+\Big\langle\frac{\delta\ell}{\delta\mathbf{z}},\,\boldsymbol{\gamma}\Big\rangle+\Big\langle\frac{\delta\ell}{\delta\rho_\psi},\,[\eta,\rho_\psi]\Big\rangle\bigg)\mathrm{d}t=0\,,$$

one writes the Euler-Poincaré equations as

$$-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta\ell}{\delta\boldsymbol{\zeta}}+\frac{\delta\ell}{\delta\phi}\mathbb{J}\boldsymbol{\zeta}+\frac{\delta\ell}{\delta\mathbf{z}}=0\,,\qquad\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta\ell}{\delta\phi}=0\,,\qquad-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta\ell}{\delta\xi}+\left[\xi,\frac{\delta\ell}{\delta\xi}\right]+\left[\rho_\psi,\frac{\delta\ell}{\delta\rho_\psi}\right]=0\,.$$

In particular, for the Lagrangian (19), we have

$$\frac{\delta\ell}{\delta\boldsymbol{\zeta}}=\mathbb{J}\mathbf{z}\,,\qquad\frac{\delta\ell}{\delta\phi}=1\,,\qquad\frac{\delta\ell}{\delta\xi}=-i\hbar\rho_\psi\,,\qquad\frac{\delta\ell}{\delta\rho_\psi}=i\hbar\xi-\widetilde{H}(\mathbf{z})\,,\qquad\frac{\delta\ell}{\delta\mathbf{z}}=-\mathbb{J}\boldsymbol{\zeta}-\langle\rho_\psi|\nabla_{\mathbf{z}}\widetilde{H}(\mathbf{z})\rangle\,,$$

such that the Euler-Poincaré equations yield

$$\begin{aligned}-\mathbb{J}\dot{\mathbf{z}}+\mathbb{J}\boldsymbol{\zeta}-\mathbb{J}\boldsymbol{\zeta}-\langle\rho_\psi|\nabla_{\mathbf{z}}\widetilde{H}(\mathbf{z})\rangle&=0\\-i\hbar\dot\rho_\psi+[\xi,-i\hbar\rho_\psi]-\Big[\rho_\psi,i\hbar\xi-\widetilde{H}(\mathbf{z})\Big]&=0\,.\end{aligned}$$

thereby completing the proof. ∎

Although based on a simple idea, the Ehrenfest mean-field model is still the most widely used model for ab initio molecular dynamics. Then, this approach is combined with other methods to improve its performance.

As we observed, expectation values play a crucial role in the derivation of the model. Most importantly, combining expectation values and coherent states returns canonical motion on the particle that is treated classically. We saw how expectation values exhibit crucial momentum map properties. Yet, much more can be said about expectation values and this is the topic of the next Sections.

4.2 Expectation values and the Ehrenfest group

In chemical physics, the expectation values of the canonical observables acquire a special meaning, especially within Ehrenfest's mean-field model. For Hamiltonian operators of physical nature, we have

$$\widehat{H}(\widehat{Q},\widehat{P})=\frac{1}{2}\widehat{P}^2+V(\widehat{Q})\,.$$

This Hamiltonian is not linear in the canonical observables and thus it does not generate coherent states, so that the expectation values possess nontrivial dynamics. Their equations are obtained from (3) and are known as ***Ehrenfest theorem***, which written in the form

$$\frac{\mathrm{d}\langle\hat{Q}\rangle}{\mathrm{d}t}=\frac{\langle\hat{P}\rangle}{m}\,,\qquad\frac{\mathrm{d}\langle\hat{P}\rangle}{\mathrm{d}t}=-\Big\langle\nabla V(\hat{Q})\Big\rangle\,,\qquad i\hbar\dot\psi=\left[\frac{1}{2}\widehat{P}^2+V(\widehat{Q})\right]\psi\,.\tag{21}$$

At this point, we quote [22]:

"These equations are often stated by saying that the expectation values follow the classical motion. This statement is in general incorrect, as may be seen by noting that [...] the force is not a function of $\langle\hat{Q}\rangle$".

Still, the question remains: what is the geometry of expectation value dynamics for arbitrary quantum systems? More specifically: what is the geometry of Ehrenfest theorem? It is clear that to address this question, we need to define our dynamics to be defined on the space $\mathbb{R}^{2n} \times \mathbf{P}\mathscr{H}$ and we just proved that this space is naturally acted on by the direct product group

$$\mathcal{H}(\mathbb{R}^{2n}, \mathbb{J}) \times \mathcal{U}(\mathscr{H})$$

The observation that hybrid classical-quantum dynamics can be expressed by using the Heisenberg and unitary groups motivates us to investigate further the interplay between these two group structures. The next Section shows that combining the two groups into a semidirect product yields the variational formulation of quantum expectation dynamics.

While the previous Section used the direct product $\mathcal{H}(\mathbb{R}^{2n}) \times \mathcal{U}(\mathscr{H})$ group structure to obtain hybrid classical-quantum dynamics, we shall now illustrate how constructing the semidirect product $\mathcal{H}(\mathbb{R}^{2n}) \circledS \mathcal{U}(\mathscr{H})$ allows to shed new light on the dynamics of expectation values, thereby extending Ehrenfest theorem to more general situations.

Definition 4.2 (Semidirect-product Lie groups) *Let G and H be two Lie groups and let $\Phi : G \times H \to H$ be a smooth left action of G on H by Lie group homomorphisms. Denote, as usual, $\Phi(g)(h) = g \cdot h$, for $g \in G$ and $h \in H$. The semidirect product group $G \circledS H$ is the manifold $G \times H$ endowed with the multiplication*

$$(g_1, h_1)(g_2, h_2) = (g_1 g_2, h_1(g_1 \cdot h_2)) \qquad \forall g_1, g_2 \in G \quad \forall h_1, h_2 \in H\,,$$

identity $e_{G \circledS H} = e_G e_H$ and inverse element

$$(g, h)^{-1} = (g^{-1}, g^{-1} \cdot h^{-1})\,.$$

The semidirect product $\mathcal{H}(\mathbb{R}^{2n}) \circledS \mathcal{U}(\mathscr{H})$ can be constructed upon using the celebrated displacement operator from the theory of coherent quantum states. This is defined as follows

$$U_h \psi(\boldsymbol{x}) = e^{-\frac{i}{\hbar}\left(\varphi + \frac{\mathbf{h}_p \cdot \mathbf{h}_q}{2} - \mathbf{h}_p \cdot \boldsymbol{x}\right)} \psi(\boldsymbol{x} - \mathbf{h}_q)\,, \qquad \forall h = (\mathbf{h}, \varphi) \in \mathcal{H}(\mathbb{R}^{2n})\,,$$

where the phase space vector $\mathbf{h} \in \mathbb{R}^{2n}$ is expressed as $\mathbf{h} = (\mathbf{h}_q, \mathbf{h}_p)$. This operator defines a group homomorphism that can be used to construct the following product rule in $\mathcal{H}(\mathbb{R}^{2n}) \circledS \mathcal{U}(\mathscr{H})$:

$$(h_1, U_1)(h_2, U_2) = \left(h_1 h_2, U_1(U_{h_1} U_2 U_{h_1}^\dagger)\right)\,, \qquad \forall h_1, h_2 \in \mathcal{H}(\mathbb{R}^{2n})\,, \quad \forall U_1, U_2 \in \mathcal{U}(\mathscr{H})\,, \tag{22}$$

where $h_1 h_2$ is the product rule in the Heisenberg group. Notice, upon denoting $\widehat{Z} = (\widehat{Q}, \widehat{P})$ (quantum canonical operators), the displacement operator U_h leads to the following Lie algebra homomorphism $\iota : \mathfrak{h}(\mathbb{R}^{2n}) \to \mathfrak{u}(\mathscr{H})$

$$\iota(\zeta) = -i\hbar^{-1}(\phi + \boldsymbol{\zeta} \cdot \mathbb{J}\widehat{Z}) = \widehat{\zeta}\,, \qquad \forall \zeta = (\boldsymbol{\zeta}, \phi) \in \mathfrak{h}(\mathbb{R}^{2n})\,,$$

which occurs in the Lie bracket structure on $\mathfrak{h}(\mathbb{R}^{2n}) \circledS \mathfrak{u}(\mathscr{H})$, given by

$$\mathrm{ad}_{(\zeta_1, \xi_1)}(\zeta_2, \xi_2) = \Big(\mathrm{ad}_{\zeta_1} \zeta_2,\ [\xi_1, \iota(\zeta_2)] - [\xi_2, \iota(\zeta_1)] + [\xi_1, \xi_2]\Big)\,,$$

where the operator 'ad' appearing in the first slot on the RHS is the infinitesimal adjoint action on $\mathfrak{h}(\mathbb{R}^{2n})$. No confusion should arise from this notation.

Here, we shall construct a dynamical theory by using the group structure above in the Lagrangian (20). To this purpose, we need to find an action of $\mathcal{H}(\mathbb{R}^{2n}) \circledS \mathcal{U}(\mathscr{H})$ on the space $\mathbb{R}^{2n} \times \mathbf{P}\mathscr{H}$. This task can be achieved by computing the coadjoint representation on the semidirect product. This computation can benefit from the following property.

Lemma 4.3 (Equivariance) *With the notation above, the following relation holds*

$$\iota(\mathrm{Ad}_h\,\zeta) = U_h\,\iota(\zeta)\,U_h^\dagger\,,$$

where $\mathrm{Ad}_h\,\zeta = (\boldsymbol{\zeta},\,\phi + \mathbf{h}\cdot\mathbb{J}\boldsymbol{\zeta})$ *is the adjoint representation on* $\mathcal{H}(\mathbb{R}^{2n})$*.*

Proof. This follows by direct substitution

$$\iota(\mathrm{Ad}_h\,\zeta) = \iota\Big(\boldsymbol{\zeta},\,\phi + \mathbf{h}\cdot\mathbb{J}\boldsymbol{\zeta}\Big) = -i\hbar^{-1}\Big(\phi + \mathbf{h}\cdot\mathbb{J}\boldsymbol{\zeta} - \widehat{Z}\cdot\mathbb{J}\boldsymbol{\zeta}\Big) = -i\hbar\left(\phi - \Big(\widehat{Z} - \mathbf{h}I\Big)\cdot\mathbb{J}\boldsymbol{\zeta}\right) =$$
$$= -i\hbar\big(\phi - (U_h\widehat{Z}U_h^\dagger)\cdot\mathbb{J}\boldsymbol{\zeta}\big) = U_h\big(-i\hbar(\phi + \mathbb{J}\widehat{Z}\cdot\boldsymbol{\zeta})\big)U_h^\dagger = U_h\,\iota(\zeta)\,U_h^\dagger\,. \qquad \blacksquare$$

Eventually, by making use of the previous relations in the definition of coadjoint representation, one finds the following expression:

$$\mathrm{Ad}^*_{(h,U)}(\nu,\mu) = \Big(\boldsymbol{\nu} - \sigma\mathbb{J}\mathbf{h} + \langle \mu - U^\dagger\mu U, i\hbar^{-1}\mathbb{J}Z\rangle,\,\sigma,\,U_h^\dagger U^\dagger \mu U U_h\Big)$$

where we have used the notation $\nu = (\boldsymbol{\nu},\sigma) \in \mathfrak{h}(\mathbb{R}^{2n})^* \simeq \mathbb{R}^{2n+1}$. This coadjoint representation is computed explicilty in the Appendix A.

Then, upon fixing the invariant set $\sigma = 1$ and by introducing the variables $\mathbf{z} = -\mathbb{J}\boldsymbol{\nu}$ and $\rho_\psi = i\hbar^{-1}\mu$, we obtain the following action of $\mathcal{H}(\mathbb{R}^{2n})\circledS\,\mathcal{U}(\mathscr{H})$ on the space $\mathbb{R}^{2n}\times\mathbf{P}\mathscr{H}$:

$$\boxed{\Phi_{(h,U)}(\mathbf{z},\rho_\psi) = \Big(\mathbf{z} - \mathbf{h} + \langle UZU^\dagger - Z\rangle,\,U_h^\dagger U^\dagger \rho_\psi U U_h\Big)\,,}$$

where we have used the expectation value notation $\langle A\rangle = \langle A|\rho_\psi\rangle$.

4.2.1 Geometry of quantum expectation dynamics

At this point, the semidirect product $\mathcal{H}(\mathbb{R}^{2n})\circledS\,\mathcal{U}(\mathscr{H})$ has been characterized and it has been showed to possess an action on the classical-quantum phase space $\mathbb{R}^{2n}\times\mathbf{P}\mathscr{H}$. Then, we consider the evolution of the classical-quantum variables $(\mathbf{z},\rho_\psi)$ under the action of (h^{-1},U^{-1}), which then gives

$$\mathbf{z}(t) = \mathbf{z}_0 + \mathbf{h}(t) + \big\langle U(t)^\dagger\widehat{Z}U(t) - \widehat{Z}\,\big|\,\rho_{\psi_0}\big\rangle\,, \qquad \rho_\psi(t) = U_h(t)U(t)\rho_{\psi_0}U(t)^\dagger U_h(t)^\dagger\,. \tag{23}$$

The evolution above has the following crucial feature:

$$\boxed{\mathbf{z}(t) - \big\langle\widehat{Z}|\rho_\psi(t)\big\rangle = \mathbf{z}_0 - \langle\widehat{Z}|\rho_{\psi_0}\rangle\,,}$$

as it is verified upon computing

$$\big\langle\widehat{Z}\,\big|\,U(t)\rho_{\psi_0}U(t)^\dagger\big\rangle = \big\langle\widehat{Z}\,\big|\,U_h(t)^\dagger\rho_\psi(t)U_h(t)\big\rangle = \big\langle U_h(t)\widehat{Z}U_h(t)^\dagger\,\big|\,\rho_\psi(t)\big\rangle = \big\langle\widehat{Z} - \mathbf{h}(t)I\,\big|\,\rho_\psi(t)\big\rangle\,.$$

Therefore, in order to study expectation value dynamics, one can simply initiate the evolution under the initial condition $\mathbf{z}_0 = \langle\widehat{Z}\,|\,\rho_{\psi_0}\rangle$, which is then replaced in (23). Moreover, the evolution above, produces the equations of motion

$$\dot{\mathbf{z}} = \boldsymbol{\zeta} - \big\langle[\rho,\widehat{Z}],\xi\big\rangle\,, \qquad \dot{\rho} = \Big[i\hbar^{-1}\widehat{Z}\cdot\mathbb{J}\boldsymbol{\zeta} + \xi,\rho\Big]$$

where $\zeta = \dot{\mathbf{h}}$ and $\xi = U_h\dot{U}U^\dagger U_h^\dagger$. Analogous expressions hold for the variations $(\delta\mathbf{z}, \delta\rho)$.

At this point, we consider the Euler-Poincaré Lagrangian of the classical-quantum mean field model (19). Although that was written previously on the space $(\mathfrak{h}(\mathbb{R}^{2n})\oplus\mathfrak{u}(\mathscr{H}))\times(\mathbb{R}^{2n}\times\mathbf{P}\mathscr{H})$, we now change perspective and we interpret the same expression (19) for $\ell(\boldsymbol{\zeta}, \phi, \xi, \mathbf{z}, \rho_\psi)$ as a Lagrangian of the type

$$\ell : \big(\mathfrak{h}(\mathbb{R}^{2n})\,Ⓢ\,\mathfrak{u}(\mathscr{H})\big) \times \big(\mathbb{R}^{2n} \times \mathbf{P}\mathscr{H}\big) \to \mathbb{R}\,.$$

Notice that the Hamiltonian operator $H(\mathbf{z})$ depends on the classical variable $\mathbf{z}$, which has to be interpreted as the expectation value $\langle\widehat{Z}|\rho_\psi\rangle$. This amounts to consider quantum systems for which the total energy can be written in terms of both the quantum state ρ_ψ and its corresponding expectation values $\mathbf{z} = \langle\widehat{Z}|\rho_\psi\rangle$. (Notice that this is a very general case, as it shown by considering the kinetic energy expression $\langle\widehat{P}^2\rangle_\psi/2 = \langle p\rangle^2/2 + \langle\widehat{P} - \langle p\rangle\rangle_\psi^2/2)$.

Theorem 4.4 *Consider the Lagrangian (19) and its associated variational principle for mixed quantum states*

$$\delta\int_{t_1}^{t_2}\Big(\phi(t) + \boldsymbol{\zeta}(t)\cdot\mathbb{J}\mathbf{z}(t) + \Big\langle\rho(t), i\hbar\xi(t) - H(\mathbf{z}(t))\Big\rangle\Big)\mathrm{d}t = 0\,,$$

with variations

$$\begin{aligned}
&\delta\boldsymbol{\zeta} = \dot{\boldsymbol{\gamma}}\,, \qquad \delta\phi = \dot{\theta} - \boldsymbol{\zeta}\cdot\mathbb{J}\boldsymbol{\gamma}\,,\\
&\delta\xi = \dot{\eta} - i\hbar^{-1}\Big(\Big[\xi, \widehat{Z}\cdot\mathbb{J}\boldsymbol{\gamma}\Big] - \Big[\eta, \widehat{Z}\cdot\mathbb{J}\boldsymbol{\zeta}\Big]\Big) + [\eta, \xi]\,,\\
&\delta\mathbf{z} = \boldsymbol{\gamma} - \big\langle[\rho, \widehat{Z}], \eta\big\rangle\,,\\
&\delta\rho = \Big[i\hbar^{-1}\widehat{Z}\cdot\mathbb{J}\boldsymbol{\gamma} + \eta, \rho\Big]\,,
\end{aligned}$$

where $(\boldsymbol{\gamma}, \theta) \in \mathfrak{h}(\mathbb{R}^{2n}, \mathbb{J})$ and $\eta \in \mathfrak{u}(\mathscr{H})$ are arbitrary and vanish at the endpoints. Then, this is equivalent to the following equations of motion

$$\dot{\mathbf{z}} = \mathbb{J}\nabla_{\mathbf{z}}\langle\rho|H(\mathbf{z})\rangle - i\hbar^{-1}\Big\langle\widehat{Z}\Big|\big[H(\mathbf{z}), \rho\big]\Big\rangle\,, \tag{24}$$

$$i\hbar\dot{\rho} = [H(\mathbf{z}), \rho] + \nabla_{\mathbf{z}}\langle\rho|H(\mathbf{z})\rangle\cdot\Big[\widehat{Z}, \rho\Big]\,. \tag{25}$$

Proof. This follows by a direct subsistution of the variations in the action principle. We have

$$\delta\int\Big(\phi(t)+\boldsymbol{\zeta}(t)\cdot\mathbb{J}\mathbf{z}(t)+\Big\langle\rho(t),i\hbar\xi(t)-H(\mathbf{z}(t))\Big\rangle\Big)\,{\rm d}t=$$
$$=\int\Big(\delta\phi+\mathbb{J}\mathbf{z}\cdot\delta\boldsymbol{\zeta}-\langle i\hbar\rho,\delta\xi\rangle-(\mathbb{J}\boldsymbol{\zeta}+\langle\rho|\nabla_{\mathbf{z}}H(\mathbf{z})\rangle)\cdot\delta\mathbf{z}+\langle i\hbar\xi-H(\mathbf{z}),\delta\rho\rangle\Big)\,{\rm d}t$$
$$=\int\Big(\dot\theta-\boldsymbol{\zeta}\cdot\mathbb{J}\boldsymbol{\gamma}+\mathbb{J}\mathbf{z}\cdot\dot{\boldsymbol{\gamma}}-\Big\langle i\hbar\rho,\dot\eta-i\hbar^{-1}\big(\Big[\xi,\widehat{Z}\cdot\mathbb{J}\boldsymbol{\gamma}\Big]-\Big[\eta,\widehat{Z}\cdot\mathbb{J}\boldsymbol{\zeta}\Big]\big)+[\eta,\xi]\Big\rangle+$$
$$-(\mathbb{J}\boldsymbol{\zeta}+\langle\rho|\nabla_{\mathbf{z}}H(\mathbf{z})\rangle)\cdot\Big(\boldsymbol{\gamma}-\langle[\rho,\widehat{Z}],\eta\rangle\Big)+\Big\langle i\hbar\xi-H(\mathbf{z}),\Big[i\hbar^{-1}\widehat{Z}\cdot\mathbb{J}\boldsymbol{\gamma}+\eta,\rho\Big]\Big\rangle\Big)\,{\rm d}t$$
$$=\int\Big(\Big\langle-\mathbb{J}\dot{\mathbf{z}}-\langle\rho|\nabla_{\mathbf{z}}H(\mathbf{z})\rangle+\Big\langle\big[i\hbar^{-1}\rho,H(\mathbf{z})\big],\mathbb{J}\widehat{Z}\Big\rangle,\boldsymbol{\gamma}\Big\rangle$$
$$+\Big\langle i\hbar\dot\rho+\Big[\rho,\widehat{Z}\cdot\langle\rho|\nabla_{\mathbf{z}}H(\mathbf{z})\rangle\Big]+[\rho,H(\mathbf{z})],\boldsymbol{\eta}\Big\rangle\Big)\,{\rm d}t$$

Then, since $\boldsymbol{\gamma}$, θ and η are arbitrary and vanish at the endpoints, the proof follows. ■

In order to understand how the above result is related to the usual Ehrenfest equations for quantum expectation dynamics, we immediately observe how these equations (21) are recovered (along with the evolution of ψ) from (24)-(25) in the case when $\nabla_{\mathbf{z}}H(\mathbf{z})=0$. As it was pointed out previously, the new feature of equations (24)-(25) lies in the fact that the expectation values have been considered as independent variables already occurring in the expression of the conserved total energy $\langle H(\mathbf{z})\rangle$. This confers the system (24)-(25) a hybrid classical-quantum structure. Indeed, one observes that new coupled classical-quantum terms appear in Ehrenfest dynamics: these are the first term on the RHS of (24) and the second term on the RHS of (25).

Notice, the first term on the RHS of (24) does not involve the quantum scales given by $\hbar$. For example, a purely classical system is given by a quantum phase-type Hamiltonian operator of the form $H(\mathbf{z})=\mathsf{h}(\mathbf{z})\mathbf{1}$, where $\mathsf{h}(\mathbf{z})$ is the classical expression of the Hamiltonian. In this case, while equation (24) recovers classical Hamilton's equations, the quantum evolution (25) specializes to coherent state dynamics of the type

$$i\hbar\dot\psi=\nabla_{\mathbf{z}}\mathsf{h}\cdot\widehat{Z}\psi.$$

This establishes how quantum states evolve under the action of purely classical degrees of freedom, thereby enlightening the interplay between classical and quantum dynamics. The same equation can also be obtained by linearizing the quantum Hamiltonian operator $H(\widehat{Z})$ around the expectation values (i.e. in the limit $\widehat{Z}\to\mathbf{z}I$), as prescribed by Littlejohn's nearby orbit approximation for semiclassical mechanics [22].

4.2.2 Coadjoint orbits on the Ehrenfest group

In this Section, we collect conclusive remarks about the structure of the equations (24)-(25). So far, the introduction of the Ehrenfest group and its use in the mean-field variational principle appeared as an artifact that recovers the Ehrenfest theorem by a fortunate coincidence. In this Section, we shall derive equations (24)-(25) from first principles without making any assumption. More particularly, we show that they are Lie Poisson on the Ehrenfest group. The present treatment follows closely the work in [5].

To get started, let us consider the Poisson bracket for the Schrödinger equation

$$\{f,h\}[\psi] = \frac{1}{2\hbar}\left\langle i\frac{\delta f}{\delta\psi}, \frac{\delta h}{\delta\psi}\right\rangle . \tag{26}$$

Now, let us write this bracket for functionals $\tilde{f}[\psi,\mathbf{z},\sigma], \tilde{g}[\psi,\mathbf{z},\sigma]$ that depend on ψ both explicitly and through the quantities

$$\sigma = \|\psi\|^2 , \qquad\qquad \mathbf{z} = \langle\psi|\widehat{Z}\psi\rangle .$$

Then, a simple chain rule calculation yields

$$\frac{\delta f}{\delta\psi} = \frac{\delta\tilde{f}}{\delta\sigma}\psi + \frac{\delta\tilde{f}}{\delta\mathbf{z}}\cdot\widehat{Z}\psi + \frac{\delta\tilde{f}}{\delta\psi}$$

thereby producing the Poisson bracket

$$\{\tilde{f},\tilde{g}\} = \sigma\{\tilde{f},\tilde{g}\}_{cl} + \frac{1}{2\hbar}\left\langle i\frac{\partial f}{\partial\psi}, \frac{\partial\tilde{g}}{\partial\psi}\right\rangle + \frac{1}{\hbar}\left\langle i\frac{\delta\tilde{f}}{\delta\psi}, \frac{\delta\tilde{g}}{\delta\mathbf{z}}\cdot\hat{Z}\psi\right\rangle - \frac{1}{\hbar}\left\langle i\frac{\delta\tilde{g}}{\delta\psi}, \frac{\delta\tilde{f}}{\delta\mathbf{z}}\cdot\hat{Z}\psi\right\rangle . \tag{27}$$

This bracket recovers (24)-(25) by using the Hamiltonian functional

$$h(\psi,\mathbf{z},\sigma) = \langle\psi, H(\mathbf{z}(t))\psi\rangle .$$

At this point, the change of variables $\mathbf{z}\mapsto\mathbb{J}\mathbf{z}$ and $\rho\mapsto -i\hbar\rho$ takes the Poisson bracket above into the Lie-Poisson on the semidirect-product Lie algebra $\mathfrak{h}(\mathbb{R}^{2n})\circledS\mathfrak{u}(\mathscr{H})$, which is the Lie algebra of the Ehrenfest group.

Thus, we have shown how the Ehrenfest group does not emerge as an artifact to capture expectation value dynamics. Rather, this semidirect-product group structure emerges naturally via the momentum map features of momentum maps.

The bracket (27) is the first example of a classical-quantum bracket that couples the canonical Poisson bracket underlying classical motion to the Lie-Poisson bracket (26) underlying quantum Schrödinger dynamics. However, notice that this Poisson bracket does not model the correlation effects occurring in the interaction of quantum and classical particles. Indeed, Poisson bracket structures modeling the backreaction of a quantum particle on a classical particle have been sought for decades and are still unknown despite several efforts [1, 3, 7, 18, 26, 28]. Rather, the Ehrenfest bracket governs the classical-quantum coupling (middle term in (27)) between expectation value dynamics (first classical term in (27)) and quantum state evolution (last term in (27)) for the same physical system.

4.2.3 Applications in chemical physics

In [29] a class of dynamical models were proposed for the motion of the expectation values

$$\langle\widehat{Z}\rangle \qquad\qquad \langle\widehat{Z}\widehat{Z}\rangle .$$

These models are based on *semiclassical approximations* [Littlejohn (1986)] and are obtained by performing certain Taylor expansions in the Ehrenfest equations (3) for $\langle\widehat{Z}\rangle$ and $\langle\widehat{Z}\widehat{Z}\rangle$, that is

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\widehat{Z}\rangle = \big\langle[\widehat{Z},\widehat{H}]\big\rangle , \qquad\qquad i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\widehat{Z}\widehat{Z}\rangle = \big\langle[\widehat{Z}\widehat{Z},\widehat{H}]\big\rangle .$$

The approximations are performed after replacing the Hamiltonian operator $\widehat{H}$ by its Taylor expansion around the expectation value $\mathbf{z} = \langle \widehat{Z} \rangle$. However, in the general case of an of order higher than 3, the model equations may break energy conservation [30]. The framework presented in this Section provides a solution to this problem. Indeed, once the expansion has been performed in the expression of the total energy $\mathsf{H} = \langle \widehat{H} \rangle$, the Hamiltonian moment equations are uniquely determined. As a consequence of the Poisson bracket structure, these equations generally differ from those in [30] thereby ensure conservation of both the total energy and uncertainty. For further details, the reader is addressed to [5].

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A Adjoint and coadjoint representations of $\mathcal{H}(\mathbb{R}^{2n})$ Ⓢ $\mathcal{U}(\mathscr{H})$

First, by using the product rule (22), one computes the explicit formula for the conjugation action of $\mathcal{H}(\mathbb{R}^{2n})$ Ⓢ $\mathcal{U}(\mathscr{H})$ on itself

$$
\begin{aligned}
\mathrm{I}_{(h_1,U_1)}(h_2,U_2) &= (h_1,U_1)(h_2,U_2)(h_1,U_1)^{-1} = \\
&= \Big((\mathbf{h}_1,\varphi_1),U_1\Big)\Big((\mathbf{h}_2,\varphi_2),U_2\Big)\Big((-\mathbf{h}_1,-\varphi_1),U_{h_1}^\dagger U_1^\dagger U_{h_1}\Big) = \\
&= \Big((\mathbf{h}_1,\varphi_1),U_1\Big)\Big((\mathbf{h}_2-\mathbf{h}_1,\varphi_2-\varphi_1-\frac{1}{2}\mathbf{h}_2\cdot\mathbb{J}\mathbf{h}_1),U_2\left(U_{h_2}(U_{h_1}^\dagger U_1^\dagger U_{h_1})U_{h_2}^\dagger\right)\Big) = \\
&= \Big((\mathbf{h}_2,\varphi_2-\mathbf{h}_2\cdot\mathbb{J}\mathbf{h}_1),\,U_1U_{h_1}U_2(U_{h_2}U_{h_1}^\dagger U_1^\dagger U_{h_1}U_{h_2}^\dagger)U_{h_1}^\dagger\Big)\,.
\end{aligned}
$$

Then, taking an arbitrary curve

$$
(\mathbf{h}_2(t),\varphi_2(t),U_2(t))\in\mathcal{H}(\mathbb{R}^{2n})\,Ⓢ\,\mathcal{U}(\mathscr{H}) \qquad \text{such that} \quad (\mathbf{h}_2(0),\varphi_2(0),U_2(0))=(0,0,\mathrm{I})\ ,
$$

and upon denoting $(\dot{\mathbf{h}}_2(0),\dot\varphi_2(0),\dot U_2(0))=(\boldsymbol{\zeta},\phi,\xi)\in\mathfrak{h}(\mathbb{R}^{2n})$ Ⓢ $\mathfrak{u}(\mathscr{H})$ and $\dot U_{h_2}(0)=\iota(\zeta)$, one defines the adjoint action of $\mathcal{H}(\mathbb{R}^{2n})$ Ⓢ $\mathcal{U}(\mathscr{H})$ on its Lie algebra as follows

$$
\begin{aligned}
\mathrm{Ad}_{(h_1,U_1)}(\zeta,\xi) &= \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\mathrm{I}_{(h_1,U_1)}(h_2(t),U_2(t)) = \\
&= \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\Big((\mathbf{h}_2(t),\varphi_2(t)-\mathbf{h}_2(t)\cdot\mathbb{J}\mathbf{h}_1),\,U_1U_{h_1}U_2(t)(U_{h_2}(t)U_{h_1}^\dagger U_1^\dagger U_{h_1}U_{h_2}^\dagger(t))U_{h_1}^\dagger\Big) = \\
&= \Big((\dot{\mathbf{h}}_2(0),\dot\varphi_2(0)-\dot{\mathbf{h}}_2(0)\cdot\mathbb{J}\mathbf{h}_1),\,U_1U_{h_1}\dot U_2(0)(U_{h_2}(0)U_{h_1}^\dagger U_1^\dagger U_{h_1}U_{h_2}^\dagger(0))U_{h_1}^\dagger+ \\
&\quad + U_1U_{h_1}U_2(0)(\dot U_{h_2}(0)U_{h_1}^\dagger U_1^\dagger U_{h_1}U_{h_2}^\dagger(0))U_{h_1}^\dagger+ \\
&\quad - U_1U_{h_1}U_2(0)(U_{h_2}(0)U_{h_1}^\dagger U_1^\dagger U_{h_1}U_{h_2}^\dagger(0)\dot U_{h_2}(0)U_{h_2}^\dagger(0))U_{h_1}^\dagger\Big) = \\
&= \Big((\boldsymbol{\zeta},\varphi-\boldsymbol{\zeta}\cdot\mathbb{J}\mathbf{h}_1),\,U_1U_{h_1}(\xi+\iota(\zeta))U_{h_1}^\dagger U_1^\dagger-U_{h_1}\iota(\zeta)U_{h_1}^\dagger\Big) = \\
&= \Big(\mathrm{Ad}_h\,\zeta,\,U_1U_{h_1}(\xi+\iota(\zeta))U_{h_1}^\dagger U_1^\dagger-\iota(\mathrm{Ad}_h\,\zeta)\Big)\,.
\end{aligned}
$$

At this point, using the notation $(\nu,\mu) = ((\boldsymbol{\nu},\sigma),\mu) \in \mathfrak{h}(\mathbb{R}^{2n})^* \times \mathfrak{u}(\mathscr{H})^* \simeq \mathbb{R}^{2n+1} \times \mathfrak{u}(\mathscr{H})^*$, one computes the coadjoint representation on $\mathcal{H}(\mathbb{R}^{2n})\,\circledS\,\mathcal{U}(\mathscr{H})$ via the pairing

$$\begin{aligned}\Big\langle \operatorname{Ad}^*_{(h,U)}(\nu,\mu),\,(\zeta,\xi)\Big\rangle &= \Big\langle(\nu,\mu),\,\operatorname{Ad}_{(h,U)}(\zeta,\xi)\Big\rangle = \\ &= \Big\langle(\nu,\mu),\,\Big(\operatorname{Ad}_h\zeta,\,U_1U_{h_1}(\xi+\iota(\zeta))U^\dagger_{h_1}U^\dagger_1 - U_{h_1}\iota(\zeta)U^\dagger_{h_1}\Big)\Big\rangle = \\ &= \Big\langle\Big(\operatorname{Ad}^*_h\nu + \iota^*\Big(U^\dagger_h(U^\dagger\mu U-\mu)U_h\Big),U^\dagger_hU^\dagger\mu U_hU_h\Big),\,(\zeta,\xi)\Big\rangle\,,\end{aligned}$$

where $\operatorname{Ad}^*_h\nu = (\boldsymbol{\nu}-\sigma\mathbb{J}\mathbf{h},\sigma)$ is the coadjoint representation on $\mathcal{H}(\mathbb{R}^{2n})$, and $\iota^*:\mathfrak{u}^*(\mathscr{H})\to\mathfrak{h}^*(\mathbb{R}^{2n})$ is the dual of the Lie algebra homomorphism generated by the displacement operator U_h, which is also computed via the pairing giving the following expression

$$\iota^*(\mu) = \Big(\langle\mu,-i\hbar^{-1}\mathbb{J}\widehat{Z}\rangle,\operatorname{Tr}(i\hbar^{-1}\mu)\Big)\,,\qquad\qquad \forall\mu\in\mathfrak{u}^*(\mathscr{H})\,.$$

By direct substitution, the coadjoint action on $\mathcal{H}(\mathbb{R}^{2n})\,\circledS\,\mathcal{U}(\mathscr{H})$ reads

$$\operatorname{Ad}^*_{(h,U)}(\nu,\mu) = \Big(\boldsymbol{\nu}-\sigma\mathbb{J}\mathbf{h}+\langle\mu-U^\dagger\mu U,i\hbar^{-1}\mathbb{J}\widehat{Z}\rangle,\,\sigma,\,U^\dagger_hU^\dagger\mu UU_h\Big)\,.$$