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Chapter 1

Classical and Quantum Conjugate Dynamics – The Interplay Between Conjugate Variables

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Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/53598

1. Introduction

There are many proposals for writing Classical and Quantum Mechanics in the same language. Some approaches use complex functions for classical probability densities [1] and other define functions of two variables from single variable quantum wave functions [2,3]. Our approach is to use the same concepts in both types of dynamics but in their own realms, not using foreign unnatural objects. In this chapter, we derive many inter relationships between conjugate variables.

1.1. Conjugate variables

An important object in Quantum Mechanics is the eigenfunctions set $\{|n>\}_{n=0}^{\infty}$ of a Hermitian operator $\hat{F}$. These eigenfunctions belong to a Hilbert space and can have several representations, like the coordinate representation $\psi_n(q)=\langle q \mid n\rangle$. The basis vector used to provide the coordinate representation, $|q>$, of the wave function are themselves eigenfunctions of the coordinate operator $\hat{Q}$ We proceed to define the classical analogue of both objects, the eigenfunction and its support.

Classical motion takes place on the associated cotangent space T^*Q with variable $z=(q,\ p)$, where q and p are n dimensional vectors representing the coordinate and momentum of point particles. We can associate to a dynamical variable $F(z)$ its eigensurface, i.e. the level set

$$\Sigma_F(f)=\{z\in T^*Q \mid F(z)=f\} \tag{1}$$

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Where f is a constant, one of the values that $F(z)$ can take. This is the set of points in phase space such that when we evaluate $F(z)$, we obtain the value f. Examples of these eigensurfaces are the constant coordinate surface, $q=X$, and the energy shell, $H(z)=E$, the surface on which the evolution of classical systems take place. These level sets are the classical analogues of the support of quantum eigenfunctions in coordinate or momentum representations.

Many dynamical variables come in pairs. These pairs of dynamical variables are related through the Poisson bracket. For a pair of conjugate variables, the Poisson bracket is equal to one. This is the case for coordinate and momentum variables, as well as for energy and time. In fact, according to Hamilton's equations of motion, and the chain rule, we have that

$$\{t,\ H\}=\sum_i\left(\frac{\partial t}{\partial q^i}\frac{\partial H}{\partial p_i}-\frac{\partial H}{\partial q^i}\frac{\partial t}{\partial p_i}\right)=\sum_i\left(\frac{dt}{dq^i}\frac{dq^i}{dt}+\frac{dp_i}{dt}\frac{dt}{dp_i}\right)=\frac{dt}{dt}=1 \tag{2}$$

Now, a point in cotangent space can be specified as the intersection of $2n$ hypersurfaces. A set of $2n$ independent, intersecting, hypersurfaces can be seen as a coordinate system in cotangent space, as is the case for the hyper surfaces obtained by fixing values of coordinate and momentum, i.e. the phase space coordinate system with an intersection at $z=(q,\ p)$. We can think of alternative coordinate systems by considering another set of conjugate dynamical variables, as is the case of energy and time.

Thus, in general, the T^*Q points can be represented as the intersection of the eigensurfaces of the pair of conjugate variables F and G,

$$\Sigma_{FG}(f,\ g)=\{z\in T^*Q\mid F(z)=f,\ \ G(z)=g\}. \tag{3}$$

A point in this set will be denoted as an abstract bra $(f,\ g\mid$, such that $(f,\ g\mid u)$ means the function $u(f,\ g)$.

We can also have marginal representations of functions in phase space by using the eigensurfaces of only one of the functions,

$$\Sigma_F(f)=\{z\in T^*Q\mid F(z)=f\},\quad \text{and}\quad \Sigma_G(g)=\{z\in T^*Q\mid G(z)=g\}.$$

A point in the set $\Sigma_F(f)[\Sigma_G(g)]$ will be denoted by the bra $(f\mid[(g\mid$ and an object like $(f\mid u)[(g\mid u)]$ will mean the $f[g]$ dependent function $u(f)[u(g)]$.

1.2. Conjugate coordinate systems

It is usual that the origin of one of the variables of a pair of conjugate variables is not well defined. This happens, for instance, with the pair of conjugate variables q and p. Even though the momentum can be well defined, the origin of the coordinate is arbitrary on the trajectory of a point particle, and it can be different for each trajectory. A coordinate system fixes the origin of coordinates for all of the momentum eigensurfaces.

http://dx.doi.org/10.5772/53598

A similar situation is found with the conjugate pair energy-time. Usually the energy is well defined in phase space but time is not. In a previous work, we have developed a method for defining a time coordinate in phase space [4]. The method takes the hypersurface $q^1 = X$, where X is fixed, as the zero time eigensurface and propagates it forward and backward in time generating that way a coordinate system for time in phase space.

Now, recall that any phase space function $G(z)$ generates a motion in phase space through a set of symplectic system of equations, a dynamical system,

$$\frac{dz}{df} = X_G, \qquad X_G = \left(\frac{\partial G}{\partial p}, \; -\frac{\partial G}{\partial q}\right), \tag{4}$$

where f is a variable with the same units as the conjugate variable $F(z)$. You can think of $G(z)$ as the Hamiltonian for a mechanical system and that f is the time. For classical systems, we are considering conjugate pairs leading to conjugate motions associated to each variable with the conjugate variable serving as the evolution parameter (see below). This will be applied to the energy-time conjugate pair. Let us derive some properties in which the two conjugate variables participate.

1.3. The interplay between conjugate variables

Some relationships between a pair of conjugate variables are derived in this section. We will deal with general $F(z)$ and $G(z)$ conjugate variables, but the results can be applied to coordinate and momentum or energy and time or to any other conjugate pair.

The magnitude of the vector field $|X_G|$ is the change of length along the f direction

$$|X_G| = \sqrt{\frac{dq^i}{df}\frac{dq^i}{df} + \frac{dp_i}{df}\frac{dp_i}{df}} = \frac{dl_F}{df}, \tag{5}$$

where $dl_F = \sqrt{(dq^i)^2 + (dp^i)^2}$ is the length element.

A unit density with the eigensurface $\Sigma_G(g)$ as support

$$(z \mid g) = \delta(z - v), \qquad v \in \Sigma_G(g) \tag{6}$$

is the classical analogue of the corresponding quantum eigenstate in coordinate $\langle q \mid g \rangle$ and momentum $\langle p \mid g \rangle$ representations. When $G(z)$ is evaluated at the points of the support of $(z \mid g)$, we get the value g. We use a bra-ket like notation to emphasise the similarity with the quantum concepts.

The overlap between a probability density with an eigenfunction of $\hat{F}$ or $\hat{G}$ provides marginal representations of a probability density,

$$\varrho(f) \coloneqq (f \mid \rho) \coloneqq \int (f \mid z)(z \mid \rho) dz = \int \delta(z - f)\rho(z) dz , \qquad f \in \sum_F (f). \tag{7}$$

$$\varrho(g) \coloneqq (g \mid \rho) \coloneqq \int (g \mid z)(z \mid \rho) dz = \int \delta(z - g)\rho(z) dz , \qquad g \in \sum_G (g). \tag{8}$$

But, a complete description of a function in T^*Q is obtained by using the two dimensions unit density $(z \mid f, g) = \delta(z - (f, g))$, the eigenfunction of a location in phase space,

$$\varrho(f, g) \coloneqq (f, g \mid \rho) \coloneqq \int (f, g \mid z)(z \mid \rho) dz = \int \delta(z - (f, g))\rho(z) dz , \qquad \left(f, g\right) \in \sum_{FG} (f, g). \tag{9}$$

In this way, we have the classical analogue of the quantum concepts of eigenfunctions of operators and the projection of vectors on them.

1.4. Conjugate motions

Two dynamical variables with a constant Poisson bracket between them induce two types of complementary motions in phase space. Let us consider two real functions $F(z)$ and $G(z)$ of points in cotangent space $z \in T^*Q$ of a mechanical system, and a unit Poisson bracket between them,

$$\{F, G\} = \frac{\partial F}{\partial q^i}\frac{\partial G}{\partial p_i} - \frac{\partial G}{\partial q^i}\frac{\partial F}{\partial p_i} = 1 , \tag{10}$$

valid on some domain $\mathsf{D} = \mathsf{D}\left(\frac{\partial F}{\partial q^i}\right) \cap \mathsf{D}\left(\frac{\partial F}{\partial q^i}\right) \cap \mathsf{D}\left(\frac{\partial F}{\partial q^i}\right) \cap \mathsf{D}\left(\frac{\partial F}{\partial q^i}\right)$, according to the considered functions F and G. The application of the chain rule to functions of p and q, and Eq. (10), suggests two ways of defining dynamical systems for functions F and G that comply with the unit Poisson bracket. One of these dynamical systems is

$$\frac{dp_i}{dF} = -\frac{\partial G}{\partial q^i} , \qquad \frac{dq^i}{dF} = \frac{\partial G}{\partial p_i} . \tag{11}$$

With these replacements, the Poisson bracket becomes the derivative of a function with respect to itself

$$\{F, G\} = \frac{\partial F}{\partial q^i}\frac{\partial q^i}{\partial F} + \frac{\partial p_i}{\partial F}\frac{\partial F}{\partial p_i} = \frac{dF}{dF} = 1 . \tag{12}$$

http://dx.doi.org/10.5772/53598

Note that F is at the same time a parameter in terms of which the motion of points in phase space is written, and also the conjugate variable to G.

We can also define other dynamical system as

$$\frac{dp_i}{dG} = \frac{\partial F}{\partial q^i}, \quad \frac{dq^i}{dG} = -\frac{\partial F}{\partial p_i}. \tag{13}$$

Now, G is the shift parameter besides of being the conjugate variable to F. This also renders the Poisson bracket to the identity

$$\{F, G\} = \frac{dp_i}{dG}\frac{\partial G}{\partial p_i} + \frac{dq^i}{dG}\frac{\partial G}{\partial q^i} = \frac{dG}{dG} = 1. \tag{14}$$

The dynamical systems and vector fields for the motions just defined are

$$\frac{dz}{dG} = X_F, \quad X_F = \left(-\frac{\partial F}{\partial p_i}, \frac{\partial F}{\partial q^i}\right), \quad \text{and} \quad \frac{dz}{dF} = X_G, \quad X_G = \left(\frac{\partial G}{\partial p_i}, -\frac{\partial G}{\partial q^i}\right) \tag{15}$$

Then, the motion along one of the F or G directions is determined by the corresponding conjugate variable. These vector fields in general are not orthogonal, nor parallel.

If the motion of phase space points is governed by the vector field (15), F remains constant because

$$\frac{dF}{dG} = \frac{\partial F}{\partial q^i}\frac{\partial q^i}{\partial G} + \frac{\partial F}{\partial p_i}\frac{\partial p_i}{\partial G} = \frac{\partial p_i}{\partial G}\frac{\partial q^i}{\partial G} - \frac{\partial q^i}{\partial G}\frac{\partial p_i}{\partial G} = 0. \tag{16}$$

In contrast, when motion occurs in the F direction, by means of Eq. (16), it is the G variable the one that remains constant because

$$\frac{dG}{dF} = \frac{\partial G}{\partial q^i}\frac{\partial q^i}{\partial F} + \frac{\partial G}{\partial p_i}\frac{\partial p_i}{\partial F} = -\frac{\partial p_i}{\partial F}\frac{\partial q^i}{\partial F} + \frac{\partial q^i}{\partial F}\frac{\partial p_i}{\partial F} = 0. \tag{17}$$

Hence, motion originated by the conjugate variables $F(z)$ and $G(z)$ occurs on the shells of constant $F(z)$ or of constant $G(z)$, respectively.

The divergence of these vector fields is zero,

$$\nabla \bullet X_F = -\frac{\partial}{\partial q^i}\frac{\partial F}{\partial p_i} + \frac{\partial}{\partial p_i}\frac{\partial F}{\partial q^i} = 0, \qquad \nabla \bullet X_G = \frac{\partial}{\partial q^i}\frac{\partial G}{\partial p_i} - \frac{\partial}{\partial p_i}\frac{\partial G}{\partial q^i} = 0. \tag{18}$$

Thus, the motions associated to each of these conjugate variables preserve the phase space area.

A constant Poisson bracket is related to the constancy of a cross product because

$$X_G \wedge X_F = \frac{dz}{dF} \wedge \frac{dz}{dG} = \begin{vmatrix} \hat{q} & \hat{p} & \hat{n} \\ \frac{\partial G}{\partial p} & -\frac{\partial G}{\partial q} & 0 \\ -\frac{\partial F}{\partial p} & \frac{\partial F}{\partial q} & 0 \end{vmatrix} = \hat{n}\left(\frac{\partial G}{\partial p}\frac{\partial F}{\partial q} - \frac{\partial G}{\partial q}\frac{\partial F}{\partial p}\right) = \hat{n}\{F, G\} . \tag{19}$$

where $\hat{n}$ is the unit vector normal to the phase space plane. Then, the magnitudes of the vector fields and the angle between them changes in such a way that the cross product remains constant when the Poisson bracket is equal to one, i.e. the cross product between conjugate vector fields is a conserved quantity.

The Jacobian for transformations from phase space coordinates to (f, g) variables is one for each type of motion:

$$J = \begin{vmatrix} \frac{\partial q}{\partial f} & \frac{\partial p}{\partial f} \\ \frac{\partial q}{\partial g} & \frac{\partial p}{\partial g} \end{vmatrix} = \begin{vmatrix} \frac{\partial G}{\partial p} & -\frac{\partial G}{\partial q} \\ \frac{\partial q}{\partial g} & \frac{\partial p}{\partial g} \end{vmatrix} = \frac{\partial G}{\partial p}\frac{\partial p}{\partial g} + \frac{\partial G}{\partial q}\frac{\partial q}{\partial g} = \frac{dG}{dg} = 1 , \tag{20}$$

and

$$J = \begin{vmatrix} \frac{\partial q}{\partial f} & \frac{\partial p}{\partial f} \\ \frac{\partial q}{\partial g} & \frac{\partial p}{\partial g} \end{vmatrix} = \begin{vmatrix} \frac{\partial q}{\partial f} & \frac{\partial p}{\partial f} \\ -\frac{\partial F}{\partial p} & \frac{\partial F}{\partial q} \end{vmatrix} = \frac{\partial F}{\partial q}\frac{\partial q}{\partial f} + \frac{\partial F}{\partial p}\frac{\partial p}{\partial f} = \frac{dF}{df} = 1 . \tag{21}$$

We have seen some properties related to the motion of phase space points caused by conjugate variables.

1.5. Poisson brackets and commutators

We now consider the use of commutators in the classical realm.

The Poisson bracket can also be written in two ways involving a *commutator.* One form is

$$\{F, G\} = \left(\frac{\partial G}{\partial p}\frac{\partial}{\partial q} - \frac{\partial G}{\partial q}\frac{\partial}{\partial p}\right)F = [\mathsf{L}_G, F] = 1 , \tag{22}$$

and the other is

$$\{F,\, G\}=\left(\frac{\partial F}{\partial q}\frac{\partial}{\partial p}-\frac{\partial F}{\partial p}\frac{\partial}{\partial q}\right)G=[\mathsf{L}_F,\, G]=1\,. \tag{23}$$

With these, we have introduced the Liouville type operators

$$\mathsf{L}_F=\frac{\partial F}{\partial q}\frac{\partial}{\partial p}-\frac{\partial F}{\partial p}\frac{\partial}{\partial q}=X_F\bullet\nabla\,,\quad \text{and } \mathsf{L}_G=\frac{\partial G}{\partial p}\frac{\partial}{\partial q}-\frac{\partial G}{\partial q}\frac{\partial}{\partial p}=X_G\bullet\nabla\,. \tag{24}$$

These are Lie derivatives in the directions of X_F and X_G, respectively. These operators generate complementary motion of functions in phase space. Note that now, we also have operators and commutators as in Quantum Mechanics.

Conserved motion of phase space functions moving along the f or g directions can be achieved with the above Liouvillian operators as

$$\frac{\partial}{\partial f}=-\mathsf{L}_G,\ \text{and}\quad \frac{\partial}{\partial g}=-\mathsf{L}_F\,. \tag{25}$$

Indeed, with the help these definitions and of the chain rule, we have that the total derivative of functions vanishes, i.e. the total amount of a function is conserved,

$$\frac{d}{df}=\frac{dq}{df}\frac{\partial}{\partial q}+\frac{dp}{df}\frac{\partial}{\partial p}+\frac{\partial}{\partial f}=\frac{dz}{df}\bullet\nabla+\frac{\partial}{\partial f}=X_G\bullet\nabla+\frac{\partial}{\partial f}=\mathsf{L}_G+\frac{\partial}{\partial f}=-\frac{\partial}{\partial f}+\frac{\partial}{\partial f}=0\,, \tag{26}$$

and

$$\frac{d}{dg}=\frac{dq}{dg}\frac{\partial}{\partial q}+\frac{dp}{dg}\frac{\partial}{\partial p}+\frac{\partial}{\partial g}=\frac{dz}{dg}\bullet\nabla+\frac{\partial}{\partial g}=X_F\bullet\nabla+\frac{\partial}{\partial g}=\mathsf{L}_F+\frac{\partial}{\partial g}=-\frac{\partial}{\partial g}+\frac{\partial}{\partial g}=0\,. \tag{27}$$

Also, note that for any function $u(z)$ of a phase space point z, we have that

$$[\mathsf{L}_F,\, u(z)]=\mathsf{L}_F u(z)=X_F\bullet\nabla u(z)=\frac{\mathrm{dz}}{\mathrm{dG}}\bullet\nabla\,\mathrm{u(z)}=-\frac{\partial}{\partial g}u(z), \tag{28}$$

and

$$[\mathsf{L}_G,\, u(z)]=\mathsf{L}_G u(z)=X_G\bullet\nabla u(z)=\frac{dz}{dF}\bullet\nabla u(z)=-\frac{\partial}{\partial f}u(z)\,, \tag{29}$$

which are the evolution equations for functions along the conjugate directions f and g. These are the classical analogues of the quantum evolution equation $\frac{d}{dt}=\frac{1}{i\hbar}[\ ,\hat{H}]$ for time dependent operators. The formal solutions to these equations are

$$u(z;g)=e^{-g\mathsf{L}_F}u(z)\,,\quad \text{and}\quad u(z;f)=e^{-f\mathsf{L}_G}u(z). \tag{30}$$

With these equations, we can now move a function $u(z)$ on T^*Q in such a way that the points of their support move according to the dynamical systems Eqs. (15) and the total amount of u is conserved.

1.6. The commutator as a derivation and its consequences

As in quantum theory, we have found commutators and there are many properties based on them, taking advantage of the fact that a commutator is a derivation.

Since the commutator is a derivation, for conjugate variables $F(z)$ and $G(z)$ we have that, for integer n,

$$\left[\mathsf{L}_G^n,\,F\right]=n\,\mathsf{L}_G^{n-1}\,,\qquad \left[\mathsf{L}_G,\,F^n\right]=n\,F^{n-1},\qquad \left[\mathsf{L}_F^n,\,G\right]=n\,\mathsf{L}_F^{n-1}\,,\qquad \left[\mathsf{L}_F,\,G^n\right]=n\,G^{n-1}\,. \tag{31}$$

Based on the above equalities, we can get translation relationships for functions on T^*Q. We first note that, for a holomorphic function $u(x)=\sum_{n=0}^{\infty}u_n x^n$,

$$\left[u(\mathsf{L}_G),\,F\right]=\left[\sum_{n=0}^{\infty}u_n\mathsf{L}_G^n,\,F\right]=\sum_{n=0}^{\infty}nu_n\mathsf{L}_G^{n-1}=u'(\mathsf{L}_G)\,. \tag{32}$$

In particular, we have that

$$\left[e^{f\mathsf{L}_G},\,F\right]=f\,e^{f\mathsf{L}_G}\,. \tag{33}$$

Then, $e^{f\mathsf{L}_G}$ is the eigenfunction of the commutator $[\,\bullet\,,\,F\,]$ with eigenvalue f.

From Eq. (32), we find that

$$u(\mathsf{L}_G)F-Fu(\mathsf{L}_G)=u'(\mathsf{L}_G). \tag{34}$$

But, if we multiply by $u^{-1}(\mathsf{L}_G)$ from the right, we arrive to

$$u(\mathsf{L}_G)F\,u^{-1}(\mathsf{L}_G)=F+u'(\mathsf{L}_G)u^{-1}(\mathsf{L}_G). \tag{35}$$

This is a generalized version of a shift of F, and the classical analogue of a generalization of the quantum Weyl relationship. A simple form of the above equality, a familiar form, is obtained with the exponential function, i.e.

$$e^{f\mathsf{L}_G}Fe^{-f\mathsf{L}_G}=F+f\,. \tag{36}$$

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This is a relationship that indicates how to translate the function $F(z)$ as an operator. When this equality is acting on the number one, we arrive at the translation property for F as a function

$$F(z;f)=\left(e^{f\,\mathsf{L}_G}F(z)\right)=F(z)\,e^{f\,\mathsf{L}_G}\,1+f\;e^{f\,\mathsf{L}_G}1=F(z)+f\;. \tag{37}$$

This implies that

$$\frac{d}{df}F(z;f)=1\,, \tag{38}$$

i.e., up to an additive constant, f is the value of $F(z)$ itself, one can be replaced by the other and actually they are the same object, with f the classical analogue of the spectrum of a quantum operator.

Continuing in a similar way, we can obtain the relationships shown in the following diagram

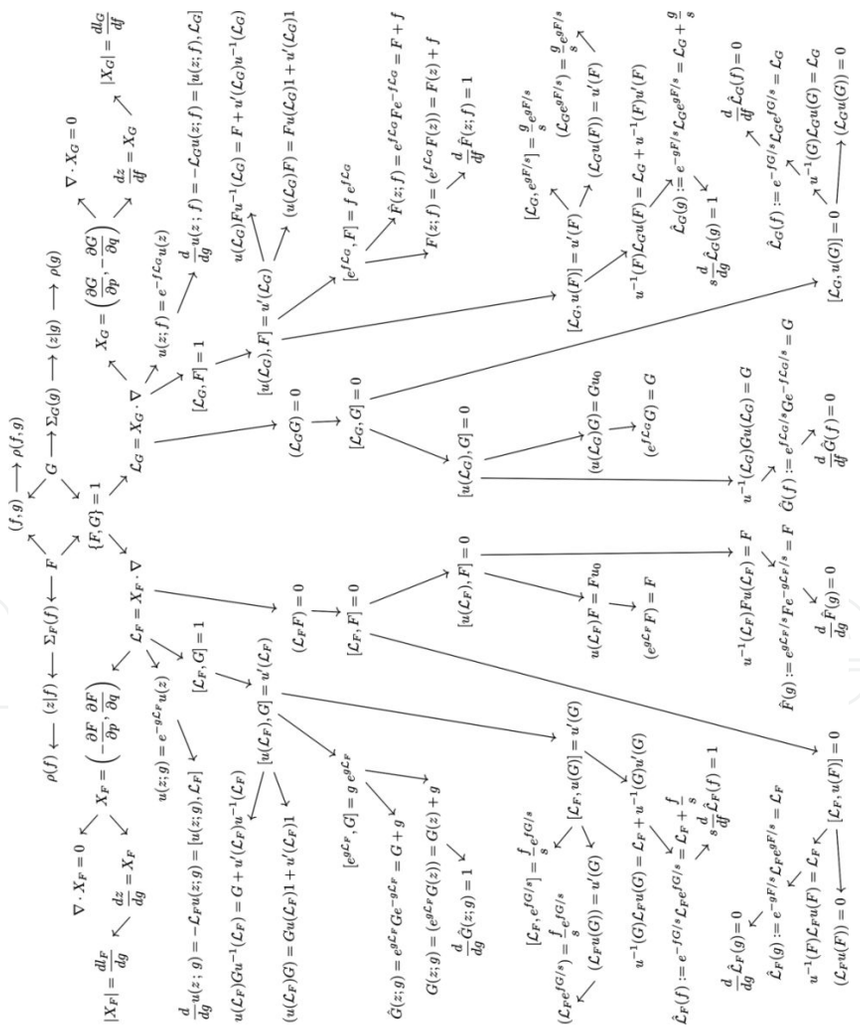


Diagram 1.

where the constant s has units of action, length times momentum, the same units as the quantum constant $\hbar$.

Some of the things to note are:

The operator $e^{g\mathsf{L}_F}$ is the eigenoperator of the commutator $[\bullet, G]$ and can be used to generate translations of $G(z)$ as an operator or as a function. This operator is also the propagator for the evolution of functions along the g direction. The variable g is more than just a shift parameter; it actually labels the values that $G(z)$ takes, the classical analogue of the spectrum of a quantum operator.

The operators L_F and $G(z)$ are also a pair of conjugate operators, as well as the pair L_G and $F(z)$.

But L_F commutes with $F(z)$ and then it cannot be used to translate functions of $F(z)$, $F(z)$ is a conserved quantity when motion occurs along the $G(z)$ direction.

The eigenfunction of $[\mathsf{L}_F, \bullet]$ and of $s\mathsf{L}_F$ is $e^{fG(z)/s}$ and this function can be used to shift L_F as an operator or as a function.

The variable f is more than just a parameter in the shift of $s\mathsf{L}_F$, it actually is the value that $s\mathsf{L}_F$ can take, the classical analogue of the spectra of a quantum operator.

The steady state of L_F is a function of $F(z)$, but $e^{gF(z)/s}$ is an eigenfunction of L_G and of $[\mathsf{L}_G, \bullet]$ and it can be used to translate L_G.

These comments involve the left hand side of the above diagram. There are similar conclusions that can be drawn by considering the right hand side of the diagram.

Remember that the above are results valid for classical systems. Below we derive the corresponding results for quantum systems.

2. Quantum systems

We now derive the quantum analogues of the relationships found in previous section. We start with a Hilbert space H of wave functions and two conjugate operators $\hat{F}$ and $\hat{G}$ acting on vectors in H, and with a constant commutator between them

$$[\hat{F}, \hat{G}] = i\hbar\,, \tag{39}$$

together with the domain $\mathsf{D} = \mathsf{D}(\hat{F}\hat{G}) \cap \mathsf{D}(\hat{G}\hat{F})$ in which the commutator holds. Examples of these operators are coordinate $\hat{Q}$ and momentum $\hat{P}$ operators, energy $\hat{H}$ and time $\hat{T}$ operators, creation $\hat{a}^{\dagger}$ and annihilation $\hat{a}$ operators.

http://dx.doi.org/10.5772/53598

The eigenvectors of the position, momentum and energy operators have been used to provide a representation of wave functions and of operators. So, in general, the eigenvectors $|f\rangle$ and $|g\rangle$ of the conjugate operators $\hat{F}$ and $\hat{G}$ provide with a set of vectors for a representation of dynamical quantities like the wave functions $\langle f \mid \psi\rangle$ and $\langle g \mid \psi\rangle$.

With the help of the properties of commutators between operators, we can see that

$$[\hat{F}^n, \hat{G}]=i\hbar\hat{F}^{n-1}, \qquad [\hat{F}, \hat{G}^n]=i\hbar\hat{G}^{n-1}. \tag{40}$$

Hence, for a holomorphic function $u(z)=\sum_{n=0}^{\infty} u_n z^n$ we have that

$$[\hat{u}(\hat{F}), \hat{G}]=i\hbar\hat{u}'(\hat{F}), \qquad [\hat{F}, \hat{u}(\hat{G})]=i\hbar\hat{u}'(\hat{G}), \tag{41}$$

i.e., the commutators behave as derivations with respect to operators. In an abuse of notation, we have that

$$\frac{1}{i\hbar}[\bullet, \hat{G}]=\frac{d\,\bullet}{d\hat{F}}, \qquad \frac{1}{i\hbar}[\hat{F}, \bullet]=\frac{d\,\bullet}{d\hat{G}}. \tag{42}$$

We can take advantage of this fact and derive the quantum versions of the equalities found in the classical realm.

A set of equalities is obtained from Eq. (43) by first writing them in expanded form as

$$\hat{u}(\hat{F})\hat{G} - \hat{G}\hat{u}(\hat{F})=i\hbar\hat{u}'(\hat{F}), \quad \text{and} \quad \hat{F}\hat{u}(\hat{G}) - \hat{u}(\hat{G})\hat{F}=i\hbar\hat{u}'(\hat{G}). \tag{43}$$

Next, we multiply these equalities by the inverse operator to the right or to the left in order to obtain

$$\hat{u}(\hat{F})\hat{G}\hat{u}^{-1}(\hat{F})=\hat{G}+i\hbar\hat{u}'(\hat{F})\hat{u}^{-1}(\hat{F}), \quad \text{and} \quad \hat{u}^{-1}(\hat{G})\hat{F}\hat{u}(\hat{G})=\hat{F}+i\hbar\hat{u}^{-1}(\hat{G})\hat{u}'(\hat{G}). \tag{44}$$

These are a set of generalized shift relationships for the operators $\hat{G}$ and $\hat{F}$. The usual shift relationships are obtained when $u(x)$ is the exponential function, i.e.

$$\hat{G}(g):=e^{-ig\hat{F}/\hbar}\hat{G}e^{ig\hat{F}/\hbar}=\hat{G}+g, \quad \text{and} \quad \hat{F}(f):=e^{if\hat{G}/\hbar}\hat{F}e^{-if\hat{G}/\hbar}=\hat{F}+f. \tag{45}$$

Now, as in Classical Mechanics, the commutator between two operators can be seen as two different derivatives introducing quantum dynamical system as

$$\frac{d\hat{P}(f)}{df} = -\frac{\partial \hat{G}(\hat{Q}, \hat{P})}{\partial Q} = \frac{1}{ih}[\hat{P}(f), \hat{G}(\hat{Q}, \hat{P})], \qquad \frac{d\hat{Q}(f)}{df} = \frac{\partial \hat{G}(\hat{Q}, \hat{P})}{\partial P} = \frac{1}{i\hbar}[\hat{Q}(f), \hat{G}(\hat{Q}, \hat{P})], \tag{46}$$

$$\frac{d\hat{P}(g)}{dg} = \frac{\partial \hat{F}(\hat{Q}, \hat{P})}{\partial Q} = \frac{1}{i\hbar}[\hat{F}(\hat{Q}, \hat{P}), \hat{P}(g)], \quad \text{and} \quad \frac{d\hat{Q}(g)}{dg} = -\frac{\partial \hat{F}(\hat{Q}, \hat{P})}{\partial P} = \frac{1}{ih}[\hat{F}(\hat{Q}, \hat{P}), \hat{Q}(g)], \tag{47}$$

where

$$\hat{P}(f) = e^{if\hat{G}/\hbar}\hat{P}e^{-if\hat{G}/\hbar}, \qquad \hat{Q}(f) = e^{if\hat{G}/\hbar}\hat{Q}e^{-if\hat{G}/\hbar}, \tag{48}$$

$$\hat{P}(g) = e^{-ig\hat{F}/\hbar}\hat{P}e^{if\hat{F}/\hbar}, \quad \text{and} \quad \hat{Q}(g) = e^{-ig\hat{F}/\hbar}\hat{Q}e^{ig\hat{F}/\hbar}. \tag{49}$$

These equations can be written in the form of a set of quantum dynamical systems

$$\frac{d\hat{z}}{df} = \hat{X}_G, \qquad \hat{X}_G = \left(\frac{\partial \hat{G}}{\partial P}, -\frac{\partial \hat{G}}{\partial Q}\right), \qquad \frac{d\hat{z}}{dg} = \hat{X}_F, \qquad \hat{X}_F = \left(-\frac{\partial \hat{F}}{\partial P}, \frac{\partial \hat{F}}{\partial Q}\right), \tag{50}$$

where $\hat{z} = (\hat{Q}, \hat{P})$.

The inner product between the operator vector fields is

$$\hat{X}_F^{\dagger} \bullet \hat{X}_F = \left(-\frac{\partial \hat{F}}{\partial P}, \frac{\partial \hat{F}}{\partial Q}\right)^{\dagger} \bullet \left(-\frac{\partial \hat{F}}{\partial P}, \frac{\partial \hat{F}}{\partial Q}\right) = \left(\frac{d\hat{Q}}{dg}\right)^2 + \left(\frac{d\hat{P}}{dg}\right)^2 := \left(\frac{d\hat{l}_F}{dg}\right)^2, \tag{51}$$

where $(d\hat{l}_F)^2 := (d\hat{Q})^2 + (d\hat{P})^2$, evaluated along the g direction, is the quantum analogue of the square of the line element $(dl_F)^2 = (dq)^2 + (dp)^2$.

We can define many of the classical quantities but now in the quantum realm. Liouville type operators are

$$\hat{\hat{\mathsf{L}}}_F := \frac{1}{i\hbar}[\hat{F}, \bullet], \quad \text{and} \quad \hat{\hat{\mathsf{L}}}_G := \frac{1}{i\hbar}[\bullet, \hat{G}]. \tag{52}$$

These operators will move functions of operators along the conjugate directions $\hat{G}$ or $\hat{F}$, respectively. This is the case when $\hat{G}$ is the Hamiltonian $\hat{H}$ of a physical system, a case in which we get the usual time evolution of operator.

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There are many equalities that can be obtained as in the classical case. The following diagram shows some of them:

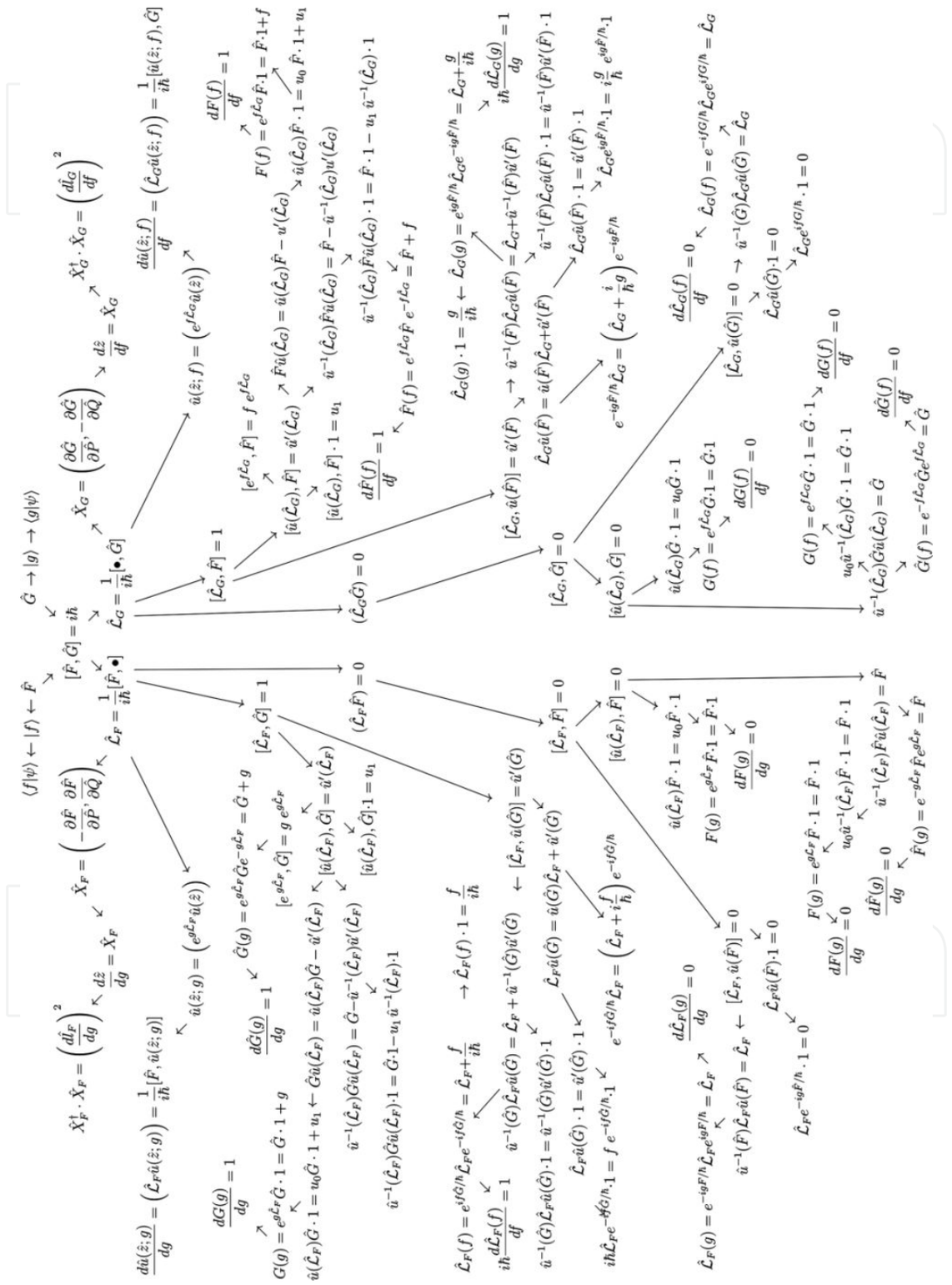


Diagram 2.

Note that the conclusions mentioned at the end of the previous section for classical systems also hold in the quantum realm.

Next, we illustrate the use of these ideas with a simple system.

3. Time evolution using energy and time eigenstates

As a brief application of the abovee ideas, we show how to use the energy-time coordinates and eigenfunctions in the reversible evolution of probability densities.

Earlier, there was an interest on the classical and semi classical analysis of energy transfer in molecules. Those studies were based on the quantum procedure of expanding wave functions in terms of energy eigenstates, after the fact that the evolution of energy eigenstates is quite simple in Quantum Mechanics because the evolution equation for a wave function $i\hbar\frac{\partial}{\partial t}|\psi>=\hat{H}|\psi>$ is linear and contains the Hamiltonian operator. In those earlier calculations, an attempt to use the eigenfunctions of a complex classical Liouville operator was made [5-8]. The results in this chapter show that the eigenfunction of the Liouville operator L_H is $e^{gT(z)}$ and that it do not seems to be a good set of functions in terms of which any other function can be written, as is the case for the eigenfunctions of the Hamiltonian operator in Quantum Mechanics. In this section, we use the time eigenstates instead.

With energy-time eigenstates the propagation of classical densities is quite simple. In order to illustrate our procedure, we will apply it to the harmonic oscillator with Hamiltonian given by (we will use dimensionless units)

$$H(z)=\frac{p^2}{2}+\frac{q^2}{2}\,. \tag{53}$$

Given and energy scaling parameter E_s and the frequency ω of the harmonic oscillator, the remaining scaling parameters are

$$p_s=\sqrt{mE_s}\,,\qquad q_s=\sqrt{\frac{E_s}{m\omega^2}}\,,\qquad t_s=\frac{1}{\omega}\,. \tag{54}$$

We need to define time eigensurfaces for our calculations. The procedure to obtain them is to take the curve $q=0$ as the zero time curve. The forward and backward propagation of the zero time curve generates the time coordinate system in phase space. The trajectory generated with the harmonic oscillator Hamiltonian is

$$q(t)=\sqrt{2E}\cos\left(t+\frac{\pi}{2}\right),\qquad p(t)=\sqrt{2E}\sin\left(t+\frac{\pi}{2}\right). \tag{55}$$

With the choice of phase we have made, $q=0$ when $t=0$, which is the requirement for an initial time curve. Then, the equation for the time curve is

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$$p = q \tan\left(t + \frac{\pi}{2}\right), \quad \text{or} \quad q = p \cot\left(t + \frac{\pi}{2}\right). \tag{56}$$

These are just straight lines passing through the origin, equivalent to the polar coordinates. The value of time on these points is t, precisely. In Fig. 1, we show both coordinate systems, the phase space coordinates (q, p), and the energy time coordinates (E, t) on the plane. This is a periodic system, so we will only consider one period in time.

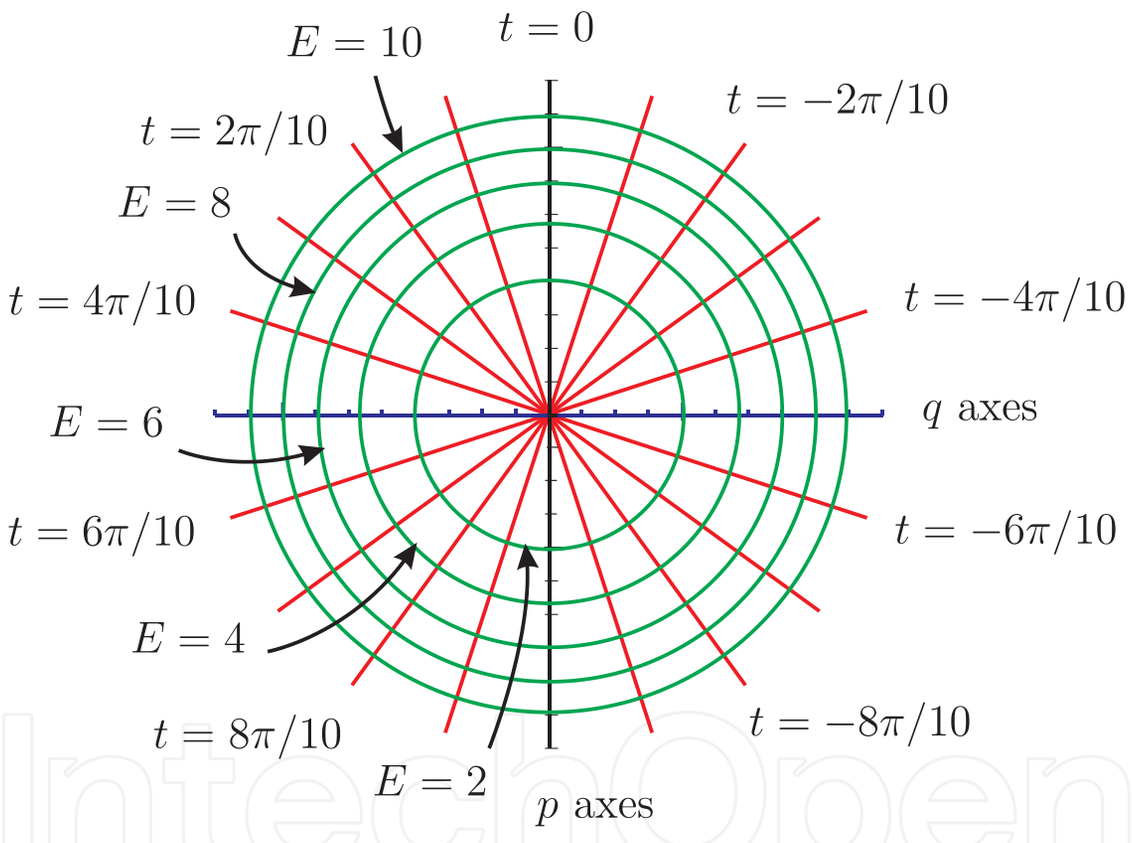


Figure 1. Two conjugate coordinate systems for the classical harmonic oscillator in dimensionless units. Blue and black lines correspond to the (q, p) coordinates and the red and green curves to the (E, t) coordinates.

At this point, there are two options for time curves. Both options will cover the plane and we can distinguish between the regions of phase space with negative or positive momentum. One is to use half lines and t in the range from $-\pi$ to π, with the curve $t=0$ coinciding with the positive p axes. The other option is to use the complete curve including positive

and negative momentum values and with $t \in (-\pi/2, \pi/2)$. In the first option, the positive momentum part of a probability density will correspond to the range $t \in (-\pi/2, \pi/2)$, and the negative values will correspond to $t \in \left(-\pi, -\frac{\pi}{2}\right) \cup \left(\pi/2, \pi\right)$. We take this option.

Now, based on the equalities derived in this chapter, we find the following relationship for a marginal density dependent only upon $H(z)$, assuming that the function $\rho(H)$ can be written as a power series of H, $\rho(H) = \sum_i \rho_i H^i$,

$$e^{-\tau \mathsf{L}_H} \rho(H) = \sum_n \frac{(-\tau)^n}{n!} \mathsf{L}_H^n \sum_i \rho_i H^i = \sum_i \rho_i H^i = \rho(H), \tag{57}$$

where we have made use of the equality $\mathsf{L}_H H = 0$. Then, a function of H does not evolve in time, it is a steady state. For a marginal function dependent upon t, we also have that

$$e^{-\tau \mathsf{L}_H} \rho(t) = e^{\tau d/dt} \rho(t) = \rho(t + \tau). \tag{58}$$

where we have made use of the result that $\frac{d}{dt} = -\mathsf{L}_H$. Therefore, a function of t is only shifted in time without changing its shape.

For a function of H and t we find that

$$e^{-\tau \mathsf{L}_H} \rho(H, t) = e^{-\tau d/dt} \rho(H, t) = \rho(H, t + \tau). \tag{59}$$

This means that evolution in energy-time space also is quite simple, it is only a shift of the function along the t axes without a change of shape.

So, let us take a concrete probability density and let us evolve it in time. The probability density, in phase space, that we will consider is

$$\rho(z) = H(z) e^{-((q-q_0)^2 + (p-p_0)^2)/2\sigma^2}, \tag{60}$$

with $(q_0, p_0) = (1,2)$ and $\sigma = 1$. A contour plot of this density in phase-space is shown in (a) of Fig. 2. The energy-time components of this density are shown in (b) of the same figure. Time evolution by an amount τ correspond to a translation along the t axes, from t to $t + \tau$, without changing the energy values. This translation is illustrated in (d) of Fig. 2 in energy-time space and in (c) of the same figure in phase-space.

Recall that the whole function $\rho(z)$ is translated in time with the propagator $e^{-\tau \mathsf{L}_H}$. Then, there are two times involved here, the variable t as a coordinate and the shift in time τ. The latter is the time variable that appears in the Liouville equation of motion $\frac{d\rho(z;\tau)}{d\tau} = -\mathsf{L}_H \rho(z;\tau)$.

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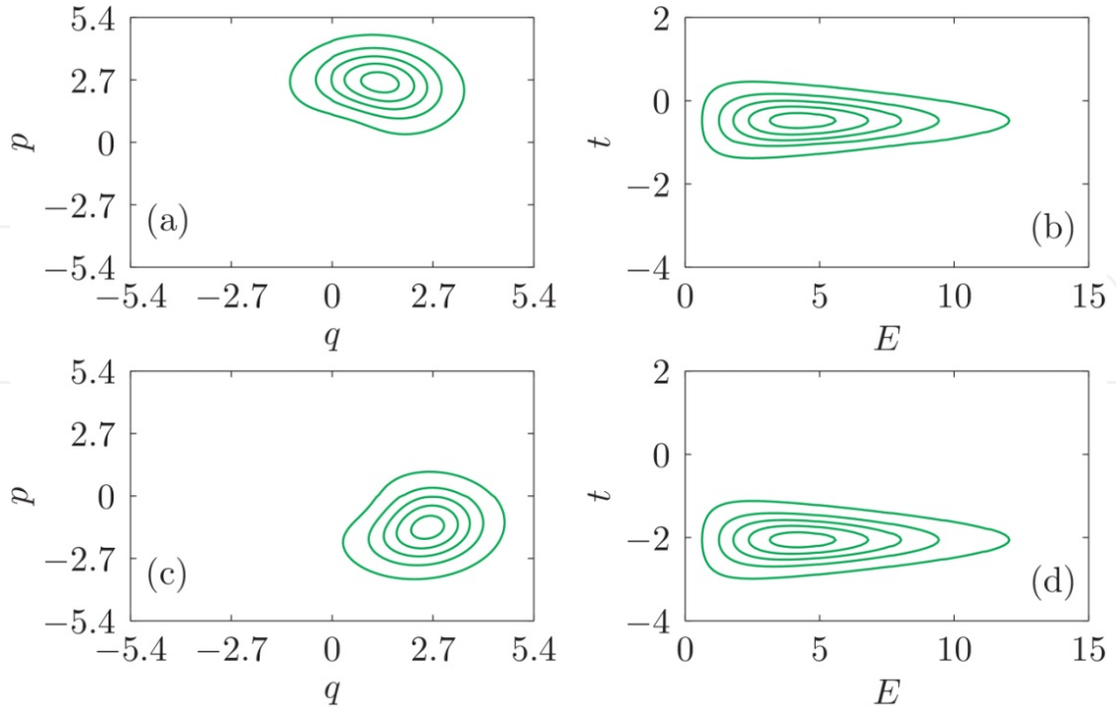


Figure 2. Contour plots of the time evolution of a probability density on phase-space and on energy-time space. Initial densities (a) in phase space, and (b) in energy-time space. (d) Evolution in energy-time space is accomplished by a shift along the *t*axes. (c) In phase space, the density is also translated to the corresponding time eigensurfaces.

This behaviour is also observed in quantum systems. Time eigenfunctions can be defined in a similar way as for classical systems. We start with a coordinate eigenfunction $|q>$ for the eigenvalue $q=0$ and propagate it in time. This will be our time eigenstate

$$|_{t>} = e^{\frac{it\hat{H}}{\hbar}} |_{q=0>} . \tag{61}$$

The projection of a wave function onto this vector is

$$<t|\psi> = <q=0|e^{-\frac{it\hat{H}}{\hbar}}|\psi> = \psi(q=0;t) , \tag{62}$$

Which is the time dependent wave function, in the coordinate representation, and evaluated at $q=0$. This function is the time component of the wave function.

The time component of a propagated wave function for a time τ is

$$<t|\psi(\tau)> = <q=0|e^{-\frac{it\hat{H}}{\hbar}} e^{-\frac{i\tau\hat{H}}{\hbar}} |\psi> = <t+\tau|\psi> . \tag{63}$$

Then, time evolution is the translation in time representation, without a change in shape. Note that the variable τ is the time variable that appears in the Schrödinger equation for the wave function.

Now, assuming a discrete energy spectrum with energy eigenvalue E_n and corresponding eigenfunction $|n>$, in the energy representation we have that

$$<n|\psi(\tau)> = <n|e^{-\frac{i\tau\hat{H}}{\hbar}}|\psi> = e^{-\frac{i\tau E_n}{\hbar}}<n|\psi> , \tag{64}$$

i.e. the wave function in energy space only changes its phase after evolution for a time τ.

4. Concluding remarks

Once that we have made use of the same concepts in both classical and quantum mechanics, it is more easy to understand quantum theory since many objects then are present in both theories.

Actually, there are many things in common for both classical and quantum systems, as is the case of the eigensurfaces and the eigenfunctions of conjugate variables, which can be used as coordinates for representing dynamical quantities.

Another benefit of knowing the influence of conjugate dynamical variables on themselves and of using the same language for both theories lies in that some puzzling things that are found in one of the theories can be analysed in the other and this helps in the understanding of the original puzzle. This is the case of the Pauli theorem [9-14] that prevents the existence of a hermitian time operator in Quantum Mechanics. The classical analogue of this puzzle is found in Reference [15].

These were some of the properties and their consequences in which both conjugate variables participate, influencing each other.

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