A geometrical description of the semi-classical limit

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Abstract

We present a general geometrical formulation for the correspondance between quantum dynamics and classical dynamics. In the projective space of quantum states, the classical dynamics is seen as an orthogonal projection of the quantum dynamics on a given family of states, such as the coherent states. This formulation is equivalent to the time-dependant-variational-principle, and thus gives a geometrical interpretation of it. Moreover the angle of this projection informs us on the validity of the approximation. These results are illustrated on a numerical example.

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1 Introduction

The relation between classical Hamiltonian dynamics and quantum Schrödinger dynamics and has first been expressed by means of the correspondence principle where classical measurable quantities are substituted by quantum operators. This relation can be understood in the Time Dependent Variational Principle (TDVP) which is an approximation scheme often used in the many body problem for example[3]. The TDVP consists in describing the quantum dynamics by Hamiltonian equations of motion on a given family of (trial) states. These equations of motions are obtained by applying the stationary phase approximation into the path integral expressed with this family of states, see [19] p.891 and [3] chap.9. In nuclear physics, these Hamiltonian equations of motion are useful to describe the collective vibrational and rotational motions of the nuclei. For a one particle problem, when applied to the standard coherent states $|qp>$ (which are Gaussian wave packets localized in phase space (q, p)), TDVP gives the classical equation of motion for the particle.

More generally coherent states are quantum states which are naturally well suited to express the quantum-classical correspondence. For that reason, they are used in many areas where quantum mechanics applies [10], as quantum optics, atomic physics, quantum field theory,...

Once we know how to associate Hamiltonian equations of motion to the Schrödinger equation of motion, the question is how properties of these different dynamics are linked. Very early, quantization rules E.B.K (Einstein-Brillouin-Keller) and W.K.B (Wentzel-Kramers-Brillouin) have been established and describe the energy spectrum starting from the classical trajectories, when the classical limit is integrable. Since the seventies, other formulas emerged as the Gutzwiller periodic orbits formula, in the more general case where the classical dynamics is chaotic or mixed [6].

For these problems, coherent states are very useful. They permit to recover the well known quantization formulas, as well as the Gutzwiller formula, by means of the description of the evolution and spreading of a single wave packets [8][7][17](Heller's lecture) [12][4]. In particular, the linearized spreading of a Gaussian wave packet can be evaluated by introducing more general coherent states known as squeezed coherent states which were first used in quantum optics.

In this paper, we will give a geometrical expression of the TDVP which links quantum and classical equations of motion. This geometrical picture is quite simple and sketched in fig.(2): we will establish, that the quantum trajectories which evolve in the space of quantum states P, give a well defined Hamiltonian dynamics on $\mathcal{S}$when projected orthogonally on a given set $\mathcal{S}$ of trial states.

The difference between the two dynamics is expressed by the angle α of the projection.

For the case of $\mathcal{S}$ being the family of coherent states ($|q, p>$) and in the semi-classical limit $\hbar \to 0$, we will find that $\alpha \sim \sqrt{\hbar}$. This means that the quantum and classical trajectories tend to be equal. The use of squeezed coherent states, permits the description of the spreading of wave-packets; it consists in dealing with an enlarged family $\mathcal{S}$. We will show that this results in $\alpha \sim \hbar$.

This angle is a measure of the validity of the classical approximation.

In the last section, we will illustrate numerically the behavior of the angle α for $\hbar \to 0$, in the case of a dynamic with one degree of freedom.

2 The classical dynamics as an orthogonal projection

Before stating the results in sections 2.3 and 2.4, we first present the major ingredients.

Suppose given a Hilbert space H containing the quantum states, and a one $\mathbb{C}-$dimensional family of vectors $|z> \in H$ parametrized by $z \in \mathbb{C}$. It is essential for the following to suppose that the family of vectors $|z>$ depends analytically on $z \in \mathbb{C}$. This family of states $|z>$ can have a special physical interest, as in the case of coherent states. It could also be parametrized by N complex variables $(z_1, z_2, .., z_N)$, but for simplicity, we will present the results for $N = 1$. Note that the vectors $|z>$ are not necessary normalized (and are in general not).

2.1 The projective space

We now need to work on the so called projective space, so we give its definition. In the Hilbert space H we decide to identify two vectors ($|\psi> \sim |\psi'>$) if they are collinear (i.e. if there exists $\lambda \in \mathbb{C}$ such that $|\psi> = \lambda|\psi'>$). We denote the equivalence class by $[\psi]$ and call it a quantum ray. This operation is natural in quantum physics because two collinear vectors evolve similarly under the (linear) Schrödinger equation and they give the same result after a measurement, so they are physically equivalent. The set of all the equivalence classes is called the projective space of the Hilbert space and is denoted by P [1].

Suppose that the family of vectors $\{|z>\}_z \subset H$ is transverse to each ray $[z]$. Then the rays define a two (real) dimensional surface $\mathcal{S} \subset P$:

$$\mathcal{S} = \{[z] \in P\}.$$

Actually $\mathcal{S}$ is a complex (one $\mathbb{C}-$dimensional) manifold. For a more general formulation we could have supposed that $\mathcal{S}$ is a given N-dimensional complex submanifold of P. To simplify, we deal in this section only with a one dimensional complex manifold (a Riemannian surface) and in local coordinates $z \in \mathbb{C}$.

Let us mention finally that as we have reduce the Hilbert space to the projective space, it seems that we have lost any possibility to describe the quantum phase. In fact, this reduction gives the Hilbert space a natural structure of a complex line bundle, with Berry's connection (or Chern's connection)[13]. We will not discuss the quantum phase here.

2.2 The Hermitian metric on P

The scalar product $< .|. >$ in the Hilbert space H induces a Hermitian metric in P and also in $\mathcal{S}$ by restriction. These spaces are called Kähler manifolds [14][16]. It means in particular that there is a Riemannian metric g and an associated symplectic two-form Ω. With the metric g we are able to measure distances between points of P and norm of tangent vectors, while the symplectic two-form Ω allows us to consider P (or $\mathcal{S}$) as a phase space to formulate Hamiltonian mechanics on it by geometrical means [2]. This metric in P is usually called the Fubiny-Study metric. There is a simple way to express the distance defined by this Riemannian metric:

The distance d between two given quantum rays $[\psi], [\phi] \in P$, represented in H by the two vectors $|\psi>$ and $|\phi>$ is [1]

$$\cos(d) = |_n < \psi|\phi >_n|^2. \tag{1}$$

Here and after, $| >_n$ means that the vector has been normalized : $|\psi >_n = |\psi > / < \psi|\psi >^{1/2}$. Remark first that the distance given by equ.(1) is indeed independent of the vectors $|\psi>$ and $|\phi>$ chosen in the rays. Secondly, the distance belongs to the interval $0 \leq d \leq \pi/2$. Two physically equivalent quantum states are represented by the same ray ($d = 0$), and two orthogonal quantum states are at the maximum distance $d = \pi/2$ from each other. Physically this distance characterizes if two quantum states are equivalent or non equivalent with respect to all possible measurements.

Infinitesimally, equ.(1) reads

$$ds^2 = 1 - |_n < \psi|\psi + d\psi >_n|^2.$$

In particular, on the Riemann surface $\mathcal{S}$, these last expressions are valid, and by developing them, we obtain that the distance between two neighbor rays $[z]$ and $[z + dz]$ is

$$
\begin{aligned}
d^2([z],[z+dz]) &= 1-|_n<z|z+dz>_n|^2 = && (2)\\
&= 1-\frac{|<z|z+dz>|^2}{<z|z><z+dz|z+dz>} && (3)\\
&= (\partial_z\partial_{\overline{z}}\ln<z|z>)\,dzd\overline{z}. && (4)
\end{aligned}
$$

The associated symplectic two-form is then expressed by [14]:

$$\Omega = i\,(\partial_z\partial_{\overline{z}}\ln<z|z>)\,dz\wedge d\overline{z}. \quad (5)$$

In these expressions, z is used as complex coordinates on $\mathcal{S}$. It would be equivalent but less convenient to use real coordinates $(q,p)\in\mathbb{R}^2$, defined for example by $z=(q+ip)/\sqrt{2}$.

Note that in equ. (2) and after, the derivation with respect to the variable z is denoted by $\partial_z\equiv\partial/\partial z$.

2.3 Equations of motion

Suppose now given a Hamiltonian $\widehat{H}$, a self-adjoint operator in H, that defines the quantum evolution by the Schrödinger equation. In this section $\hbar$ is fixed, and we do not consider the semi-classical limit $\hbar\to0$ for the moment.

We will now concentrate on what happens near the surface $\mathcal{S}$. A given quantum state $|z>$ from the surface evolves as

$$|\psi(t)>=e^{-i\widehat{H}t/\hbar}|z>.$$

By multiplying each side by a complex number $\lambda\in\mathbb{C}$, we see that the evolution is not affected, and so there is a well defined quantum trajectory $[\psi(t)]$ in the projective space P. This trajectory passes through $[z]\in\mathcal{S}$ for $t=0$ and generally leaves the surface. This is sketched on fig.(1).

We call $\vec{v}$ the velocity vector of this trajectory at the point $[z]=[\psi(0)]\in P$. We are working now in the tangent space at the point $[z]\in\mathcal{S}$. Because of the Riemannian metric g in P, it makes sense to project orthogonally this vector on the surface $\mathcal{S}$. We call $\vec{V}$ the result vector and $(\dot{z},\dot{\overline{z}})$ its coordinates on the surface $\mathcal{S}$. See fig.(1). The task now is to calculate this projected vector $\vec{V}$ and express its coordinates from the Hamiltonian $\widehat{H}$ and the Hermitian metric.

Let us note

$$\mathcal{H}(z,\overline{z}) =_n< z|\widehat{H}|z >_n . \tag{6}$$

It is a well defined function on $\mathcal{S}$, named the Q-symbol or the Normal symbol of $\widehat{H}$ [19].

We consider first an arbitrary vector $\vec{V}$ tangent to $\mathcal{S}$ with coordinates $(\dot{z},\dot{\overline{z}})$. With a limited development, and using equ. (2), we obtain that for $dt \to 0$, the distance between the extremities of vectors $\overrightarrow{v}dt$ and $\overrightarrow{V}dt$ is

$$\begin{aligned} d^2 &= d([\psi(dt)],[z+dz])^2 \qquad (7)\\ &= dt^2\left(\Delta E^2 + (\partial_{\overline{z}}\partial_z \ln < z|z >)\ \dot{z}\dot{\overline{z}} - i\ \dot{z}\ (\partial_z\mathcal{H}) + i\ \dot{\overline{z}}\ (\partial_{\overline{z}}\mathcal{H})\right) + o(dt^2), \end{aligned}$$

where $dz = \dot{z}\ dt$ and $\Delta E^2 =_n< \psi|\widehat{H}^2|\psi >_n -_n < \psi|\widehat{H}|\psi >_n^2$.

We can minimize this distance with a good choice of $\overrightarrow{V}$. This corresponds to the orthogonal projection of $\overrightarrow{v}$. Its coordinates $(\dot{z},\dot{\overline{z}})$ must verify $\partial(d^2)/\partial\dot{z} = \partial(d^2)/\partial\ \dot{\overline{z}}= 0$. From equ.(7) this gives

$$\dot{z}\ (\partial_z\partial_{\overline{z}} \ln < z|z >) = -\frac{i}{\hbar}\partial_{\overline{z}}\mathcal{H}, \tag{8}$$

together with the complex conjugate equation.

We can make the same projection for every point $[z]$ in the surface S. This gives a smooth vector field on S expressed by its coordinates $(\dot{z},\dot{\overline{z}})$. See fig.(2)

In fact the equation equ. (8) is the well known Hamilton equations of motion with Hamiltonian $\mathcal{H}$, written in complex coordinates. In the next section this equation will have the standard canonical form equ.(18). The geometrical (coordinates-independent) formulation of this Hamiltonian vector field $\overrightarrow{V}$ with symplectic form Ω on S considered as a classical phase space is [2]

$$\iota_{\overrightarrow{V}}(\Omega) = \frac{1}{2\hbar}d\mathcal{H},$$

where $\iota_{\overrightarrow{V}}$ is the interior product, and $d\mathcal{H}$ is the differential of $\mathcal{H}$.

Let us resume the main result of this paragraph: *The orthogonal projection of the quantum flow on the surface $\mathcal{S}$ gives a well defined Hamiltonian flow on $\mathcal{S}$ with Hamilton function $\mathcal{H} =_n < z|\widehat{H}|z >_n$.*

We obtain the same Hamiltonian equation of motion by applying the Time-Dependant-Variational-Principle (TDVP) to the family of states $|z>$, $z \in \mathbb{C}$. Our derivation is thus equivalent to the TDVP statement and gives a geometrical interpretation of it. The TDVP is usually expressed by using the stationary phase approximation in coherent state path integral, see [19] p.891, and [3] chap 9.

The orthogonal projection means that the Hamiltonian trajectory obtained on the phase space S are the best trajectories which approximate the exact quantum trajectories for short times evolution, with respect to the quantum distance equ.(1)

2.4 Evaluation of the approximation

It may be interesting now to evaluate quantitatively this approximation. It is represented by the angle α that the quantum trajectory makes with the surface $\mathcal{S}$, see fig.(1). To evaluate this angle, we will use a result obtained by Aharonov and Anandan [1]. They have shown by a development similar to equ.(7) that the velocity v of the quantum trajectory $[\psi(t)]$ in P is proportional to the energy incertitude of one of its states. Indeed from

$$|\psi(dt)>_n = \exp(-i\frac{\hat{H}dt}{\hbar})|\psi(0)>_n = (1 - i\frac{\hat{H}dt}{\hbar} - \frac{1}{2}\frac{\hat{H}^2 dt^2}{\hbar^2})|\psi(0)>_n + o(dt^2),$$

and from equ.(2), we obtain

$$\begin{aligned} ds^2 &= d^2([\psi(0)],[\psi(t)]) = 1 - |\,{}_n<\psi(0)|\psi(t)>_n|^2 \\ &= \frac{\Delta E^2}{\hbar^2}dt^2 + o(dt^2), \end{aligned}$$

so

$$v = \left\| \overrightarrow{v} \right\| = \frac{ds}{dt} = \frac{\Delta E}{\hbar}.$$

On the other hand, from equ.(2) and equ.(8), the velocity V on the surface S is given by

$$V^2 = (\partial_z \partial_{\bar{z}} \ln <z|z>)\dot{z}\,\dot{\bar{z}} = \frac{|\partial_z \mathcal{H}|^2}{\hbar^2(\partial_z \partial_{\bar{z}} \ln <z|z>)}.$$

The angle α is then determined by:

$$\cos^2(\alpha) = \frac{V^2}{v^2} = \frac{|\partial_z \mathcal{H}|^2}{(\Delta E)^2 (\partial_z \partial_{\bar{z}} \ln <z|z>)},$$

or

$$\alpha = \arctan \left(\frac{(\Delta E)^2 \left(\partial_z \partial_{\bar{z}} \ln < z|z > \right) - |\partial_z \mathcal{H}|^2}{|\partial_z \mathcal{H}|^2} \right)^{1/2}, \tag{9}$$

provided that $v \neq 0$. Note that $v = 0$ corresponds to a stationary quantum state $[z]$, because $\Delta E = 0$.

If $V = 0$ then $\alpha = \pi/2$, and $\partial_z \mathcal{H} = 0$. This means that if the quantum trajectory is perpendicular to the surface S, there is a fixed point in the classical trajectory. See fig.(2).

We can remark that we have approximated the evolution in the projective space but we have a priori no information about he quantum phase. This is not true in fact, and "the best" quantum phase associated to the classical trajectory $[z(t)]$, is obtained by a projection on S but this time in the Hilbert space H. This phase can be retrieved as shown by Littlejohn[11] as the sum of a dynamical phase and the geometrical Berry's phase. This phase can be useful for later re-quantization of the Hamiltonian dynamics.

In the next sections, we will apply the projection formula for different families of coherent states $\{|z>\}_z$. The interest will rest on the property that the angle α is proportional to $\sqrt{\hbar}$ or $\hbar$. This result will be interpreted by the fact that in these cases the quantum trajectory $[\psi(t)]$ becomes more and more tangential to the classical phase space S in the semi-classical limit $\hbar \to 0$.

3 Projection on the standard coherent states family

3.1 Definition and properties

In this section we will apply the formalism presented above to the family of standard coherent states (still in one degree of freedom for simplicity) [19]. We present here a short description of them. A standard coherent state $|q,p>$ is a Gaussian wave packet in $H = L^2(\mathbb{R})$ parametrized by its mean position $q =< q,p|\widehat{q}|q,p>$ and its mean impulsion $p =< q,p|\widehat{p}|q,p>$. Its wave function is :

$$\psi_{q,p}(x) =< x|q,p >= \left(\frac{1}{\pi\hbar}\right)^{1/4} \exp\left(\frac{ipx}{\hbar}\right) \exp\left(-\frac{(x-q)^2}{2\hbar}\right) \exp\left(-\frac{iqp}{2\hbar}\right) \tag{10}$$

To apply the projection of the preceding section, we need a holomorphic parametrization of the coherent states. Such an expression is well known and has been generalized to define coherent states associated to arbitrary Lie groups[15]. In our case the Lie algebra is the so called Weyl algebra. If we define the operators

$$a = \frac{1}{\sqrt{2\hbar}}(\widehat{q} + i\widehat{p}), \qquad a^+ = \frac{1}{\sqrt{2\hbar}}(\widehat{q} - i\widehat{p}),$$

they verify : $[a, a^+] = 1$.

Consider the coherent state with null mean position and null mean impulsion

$$|0 >= |q = 0, p = 0 >,$$

and define

$$|z >= e^{za^+}|0> . \tag{11}$$

with $z \in \mathbb{C}$. The family of vectors $|z >$ depends analytically on z as we wanted. With a short calculation one may verify that they coincide with the coherent states defined above, but are not normalized: $|z>_n = |z > / < z|z >^{1/2} = |q, p >$ with

$$z = \frac{1}{\sqrt{2\hbar}}(q + ip). \tag{12}$$

So in the projective space P, the surface S is defined as the set of all the rays $[z]$ of the coherent states and corresponds to the usual classical phase space, parametrized by the position and impulsion, $(q, p) \in \mathbb{R}^2$.

3.2 The Hermitian metric

The norm of a coherent state $|z >$ is [19] $< z|z >= e^{z\overline{z}}$, so $\partial_z \partial_{\overline{z}} \ln < z|z >= 1$. From equ. (2) and equ. (5), we deduce the expression of the Riemannian metric g and the symplectic two form Ω on $\mathcal{S}$ in complex coordinates z and real coordinates (q, p)

$$g = |dz|^2 = \frac{1}{2\hbar}(dq^2 + dp^2), \tag{13}$$
$$\Omega = i dz \wedge d\overline{z} = \frac{1}{\hbar} dq \wedge dp.$$

This shows that $\mathcal{S}$ is isometric to the euclidean plane. With respect to the metric g, equ.(13) shows that the distance between to fixed classical points (q,p) and (q',p') tends to infinity as $\hbar \to 0$. For that reason we renormalize the Hermitian metric and define :

$$\widetilde{g} = \frac{1}{\hbar} g, \quad \widetilde{\Omega} = \frac{1}{\hbar}\Omega \tag{14}$$

We define also the "classical" complex coordinate on $\mathcal{S}$ by

$$\mathcal{Z} = z\sqrt{\hbar} = \frac{1}{\sqrt{2}}(q + ip), \tag{15}$$

for which:

$$\widetilde{g} = \frac{1}{2}(dq^2 + dp^2) = |d\mathcal{Z}|^2 . \tag{16}$$

3.3 Projection on the surface

The projection method described in section 2.3 when applied to the standard coherent states, gives a Hamiltonian vector field V on the surface $\mathcal{S}$ (see equ.2) whose Hamiltonian is equ.(6)

$$\mathcal{H}_N(z,\overline{z}) = {}_n< z|\widehat{H}|z >_n = {}_n< qp|\widehat{H}|qp >_n = \mathcal{H}_N(q,p). \tag{17}$$

From equ. (8), equation of motion are

$$\frac{dz}{dt} = -\frac{i}{\hbar}\partial_{\overline{z}}\mathcal{H}_N(z,\overline{z}).$$

These Hamilton equations are more familiar in real coordinates (q,p),equ. (12)

$$\begin{cases} \partial_t q = \partial_p \mathcal{H}_N(q,p) \\ \partial_t p = -\partial_q \mathcal{H}_N(q,p) \end{cases} . \tag{18}$$

The Hamiltonian function equ.(17) can depend on $\hbar$. For $\hbar \to 0$, its limit (if defined) is called the classical symbol and will be denoted by $\mathcal{H}_{cl}(q,p)$.

$$\mathcal{H}_{cl}(q,p) = \lim_{\hbar \to 0} \mathcal{H}_N(q,p).$$

In this case, often encountered in practice, we can make the important following remark. For $\hbar \to 0$, consider the distance d' covered by a classical trajectory on the surface $\mathcal{S}$, over a finite time t of order 1. Then d' is of order $1/\sqrt{\hbar}$ with respect to the primitive metric g, but is of order 1 with respect to the metric $\widetilde{g}$ defined by equ.(16), see fig.(3).

3.4 Angle of projection

From its general expression equ. (9), we can calculate the angle α at each point $[z]$ of the phase space. We recall that this angle measures how fast the exact quantum trajectory differs from the classical one, see fig.(2). Expressed differently, this angle measures the rate of deformation of an initial wave packet (a coherent state belonging to $\mathcal{S}$) under evolution.

We need first an evaluation of the energy incertitude ΔE of a coherent state $|z\gg_n$. Let us first begin with the coherent state $|0\gg_n$. From equ.(11)

$$\partial_z^n |z>= a^{+n}|z> .$$

Then, we use the usual basis $|n\gg_n$, $n \in \mathbb{N}$ of the Hilbert space, defined by :

$$|n\gg_n = \frac{1}{\sqrt{n!}} a^{+n}|0> .$$

So :

$$\begin{aligned} <0|\widehat{H}^2|0>= & \sum_{n=0}^{\infty} <0|\widehat{H}|n><n|\widehat{H}|0> \\ = & \sum_{n=0}^{\infty} \frac{1}{n!} | <0|\widehat{H}a^{+n}|0> |^2 \\ = & \sum_{n=0}^{\infty} \frac{1}{n!} |\partial_z^n <z|\widehat{H}|z> |^2_{z=0}. \end{aligned}$$

But it can be verified that:

$$\forall n,\ \partial_z^n <z|\widehat{H}|z>_{/z=0} = \partial_z^n\ {}_n\!\ll z|\widehat{H}|z\gg_{n\ /z=0},$$

so

$$<0|\widehat{H}^2|0>= \sum_{n=0}^{\infty} \frac{1}{n!} |\partial_z^n\ {}_n\!\ll z|\widehat{H}|z\gg_n |^2_{z=0}. \qquad (19)$$

Let us define the translation operator

$$D(z) = e^{za^+ - \overline{z}a},$$

which acts on a coherent state as

$$D(z')|z\rangle_n = e^{iIm(z'\overline{z})}|z'+z\rangle_n \,. \tag{20}$$

We then apply equ.(19) to the operator $\widehat{H}' = D^+(z')\widehat{H}D(z')$, and obtain

$$\begin{aligned}
\partial_z^n \;{}_n\langle z|\widehat{H}'|z\rangle_{n\,/z=0} &= \partial_z^n \;{}_n\langle z|D^+(z')\widehat{H}D(z')|z\rangle_{n\,/z=0} \\
&= \partial_z^n \;{}_n\langle z+z'|\widehat{H}|z+z'\rangle_{n\,/z=0} \\
&= \partial_{z''}^n \;{}_n\langle z''|\widehat{H}|z''\rangle_{n\,/z''=z'}.
\end{aligned}$$

Then

$${}_n\langle z|\widehat{H}^2|z\rangle_n = \sum_{n=0}^{\infty} \frac{1}{n!} |\partial_{z'}^n \;{}_n\langle z'|\widehat{H}|z'\rangle_n|^2_{z'=z}.$$

This last equation is known as Moyal formula [12]. In classical variables equ.(12) we have

$${}_n < \mathcal{Z}|\hat{H}^2|\mathcal{Z} >_n = \sum_{n=0}^{\infty} \frac{\hbar^n}{n!} |\partial_{\mathcal{Z}'}^n \;{}_n\langle \mathcal{Z}'|\widehat{H}|\mathcal{Z}'\rangle_n|^2_{\mathcal{Z}'=\mathcal{Z}},$$

and finally

$$\Delta E^2 = {}_n< \mathcal{Z}|\hat{H}^2|\mathcal{Z} >_n - {}_n < \mathcal{Z}|\hat{H}|\mathcal{Z} >_n^2 = \hbar\,|\partial_{\mathcal{Z}}\mathcal{H}_N|^2 + \frac{\hbar^2}{2!}\left|\partial_{\mathcal{Z}}^2\mathcal{H}_N\right|^2 + ...$$

With equ.(9), this gives

$$\alpha = \arctan\left(\sqrt{\sum_{n\geq 2} \frac{\hbar^{n-1}|\partial_{\mathcal{Z}}^n\mathcal{H}_N|^2}{n!|\partial_{\mathcal{Z}}\mathcal{H}_N|^2}}\right),$$

except for classical fixed points where $\partial_{\mathcal{Z}}\mathcal{H}_{cl} = 0$. The derivatives are evaluated at point $[z]$.

In the semi-classical limit $\hbar \to 0$

$$\alpha = \sqrt{\frac{\hbar}{2}\frac{|\partial_{\mathcal{Z}}^2\mathcal{H}_{cl}|}{|\partial_{\mathcal{Z}}\mathcal{H}_{cl}|}} + o(\hbar^{1/2}). \tag{21}$$

This last expression diverges if $[z]$ is a fixed point for which $|\partial_z \mathcal{H}_{cl}| = 0$ and $\alpha = \pi/2$, as discussed previously. Elsewhere, the angle tends to zero as $\sqrt{\hbar}$. It means that *every quantum trajectory tends to be tangent to the phase space surface $\mathcal{S}$ in the semi-classical limit. This is the geometrical sense of the semi-classical limit.*

The angle equ.(21) is also proportional to $|\partial^2_{\mathcal{Z}} \mathcal{H}_{cl}|$, a term of the Hessian of the Hamiltonian and responsible for the deformation of the wave packet in first order [12].

The proximity between the exact quantum state $[\psi(t)]$ and the evolved coherent state $[z(t)]$ is valid for short times, but we don't expect it for longer times even for times of order unity $t \sim 1$ (which could be the period of a closed trajectory of the classical dynamics). This is because over $t \sim 1$, we have seen that the length of the trajectory is of order $1/\sqrt{\hbar}$, while the angle α is of order $\sqrt{\hbar}$. The distance $d = d([\psi(t)], [z(t)])$ can then not tend to zero, see fig.(3), but instead

$$d([\psi(t)], [z(t)]) \sim C\sqrt{\hbar}(L/\sqrt{\hbar}) \sim CL, \tag{22}$$

where C is a constant.

In the next section, it will become apparent that this distance d is mainly due to the elliptical deformation of the wave packet. Indeed, by introducing the family of squeezed coherent states, we will reduce the angle to $\alpha \sim \hbar$, and so the distance d after a finite time of order unity $t \sim 1$ will behave as $d \sim \sqrt{\hbar}$.

4 Projection on the squeezed coherent states family

The squeezed coherent states is an enlarged family of standard coherent states. Their evolution has been studied in details in [8][7][17](Heller's lecture) [12][4].For a one degree of freedom dynamics, there is a variable $R \in \mathbb{C}$ which determines the elliptic shape of the wave packet in phase space, in addition to $z \equiv (q, p)$ which specifies its position in phase space. This family of squeezed coherent states are extremely useful in quantum optics, and also in nuclear physics, and more generally in the "many-body problem", where they introduce the concept of "quasi-particles".

A Detailed mathematical presentation can be found in [19] or [15]. The holomorphic expression analogous to equ.(11) is now

$$|R, r >= \exp(\frac{R}{2}a^{+2} + ra^{+})|0 >, \tag{23}$$

with $r, R \in \mathbb{C}$. The surface $\mathcal{S}$, is now a 2-dimensional complex manifold in P. The standard coherent states is the submanifold $R = 0$.

As stated previously, the orthogonal projection of the quantum dynamics on the surface $\mathcal{S}$,will gives Hamiltonian equation of motion for the parameters r and R. These equations are those obtained by the usual TDVP and studied in details in [12][17](Heller's lecture).

Hereafter we will only give the calculation of the angle α in this case, from the general expression equ.(9). To simplify, the calculation is done at the point of $\mathcal{S}$ with coordinates $r = R = 0$.

At first order in r and R, we have

$$\begin{aligned}
|R, r &> = (1 + \frac{R}{2}a^{+2} + ra^{+})|0 > + o(r, R),\\
\partial_r |R, r &> = a^{+}|0 >,\\
\partial_R |R, r &> = \frac{1}{2}a^{+2}|0 >,\\
&< R, r|R, r >= 1 + r\bar{r} + \frac{1}{2}R\bar{R} + o(r^2, R^2),\\
\mathcal{H} &= {}_n\!< R, r|\widehat{H}|R, r >_n = < R, r|\widehat{H}|R, r > + o(r, R).
\end{aligned}$$

Let us consider

$$\begin{aligned}
D &= \begin{pmatrix} R \\ r \end{pmatrix},\\
\mathcal{M} &= (\partial_{\bar{D}}\partial_{D^t} \ln < R, r|R, r >)^{-1} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{pmatrix}.
\end{aligned}$$

Then

$$\begin{aligned}
< &\ 0|\widehat{H}^2|0 >= \sum_{n=0}^{\infty} < 0|\widehat{H}|n >< n|\widehat{H}|0 >\\
= &\ \sum_{n=0}^{\infty} \frac{1}{n!}| < 0|\widehat{H}a^{+n}|0 > |^2
\end{aligned}$$

$$
\begin{aligned}
&= \; <0|\widehat{H}|0>^2 + \left|\partial_r < R,r|\widehat{H}|R,r>\right|^2 + 2\left|\partial_R < R,r|\widehat{H}|R,r>\right|^2 \\
&\quad + \sum_{n=3}^{\infty} \frac{1}{n!} \left|\partial_r^n < R,r|\widehat{H}|R,r>\right|^2 .
\end{aligned}
$$

So

$$
\begin{aligned}
\Delta E^2 &= \; <0|\widehat{H}^2|0> - <0|\widehat{H}|0>^2 \\
&= (\partial_{D^t}\mathcal{H})\mathcal{M}(\partial_{\bar{D}}\mathcal{H}) + \sum_{n=3}^{\infty} \frac{1}{n!} \left|\partial_r^n < R,r|\widehat{H}|R,r>\right|^2_{(R,r)=(0,0)} .
\end{aligned}
$$

The angle α is then

$$
\alpha = \arctan\left(\frac{\sum_{n=3}^{\infty}\frac{1}{n!}\left|\partial_r^n\mathcal{H}\right|^2}{(\partial_{D^t}\mathcal{H})\mathcal{M}(\partial_{\bar{D}}\mathcal{H})}\right)^{1/2} . \tag{24}
$$

If we are interested in the semi-classical limit, as in equ.(15), we introduce the classical coordinate $\mathcal{Z} = \sqrt{\hbar} r$.

Then

$$
\partial_R|Rr> = \frac{1}{2}\partial_r^2|R,r> = \frac{\hbar}{2}\partial_{\mathcal{Z}}^2|R,r>,
$$

so

$$
\begin{aligned}
(\partial_{D^t}\mathcal{H})\mathcal{M}(\partial_{\bar{D}}\mathcal{H}) &= \frac{1}{2}\left|\partial_R\mathcal{H}\right|^2 + \left|\partial_r\mathcal{H}\right|^2 \\
&= \frac{\hbar^2}{8}\left|\partial_{\mathcal{Z}}^2\mathcal{H}\right|^2 + \hbar\left|\partial_{\mathcal{Z}}\mathcal{H}\right|^2 ,
\end{aligned}
$$

and

$$
\alpha = \frac{\hbar}{\sqrt{6}}\frac{|\partial_{\mathcal{Z}}^3\mathcal{H}|}{|\partial_{\mathcal{Z}}\mathcal{H}|} + o(\hbar). \tag{25}
$$

This result has been obtained for the point $R = r = 0$ of $\mathcal{S}$, but a similar expression could be obtained for any point of $\mathcal{S}$. This is because $\mathcal{S}$ is a symmetric space [19], and every point is equivalent to $R = r = 0$, by a group transformation, generalizing the translation operator equ.(20). A general expression of α can be found in [5].

In comparison to equ.(21), one order of magnitude in $\sqrt{\hbar}$ has been reached. This is sufficient now for the distance $d([\psi(t)], [R(t), r(t)])$ in fig.(3) to tend to zero (for $t \sim 1$ fixed and $\hbar \to 0$).

Intuitively, this is because

$$d([\psi(t)],[|R(t),r(t)>]) \approx \hbar\left(\frac{L}{\sqrt{\hbar}}\right) \approx \sqrt{\hbar}. \tag{26}$$

But this last estimation is not rigorous. Indeed we have to show that the quantum flow does not diverge outside the surface $\mathcal{S}$. And this is essentially due to the fact that the quantum flow is an isometry in P as shown in the demonstration of equ.(26) which follows.

The fact that the angle between the surface $\mathcal{S}$ and the flow $[\psi(t)]$ is α, is expressed by

$$d_l = \tan(\alpha_z) l + o(l), \text{ for } l \to 0,$$

where d_l is the distance between $[\psi(t)]$ and $[z(t)]$. Suppose that this is true uniformally on the surface $\mathcal{S}$, at least on a domain of interest:

$$\exists\ l_0 \text{ such that } \forall\ z,\ d_l < 2\tan(\alpha_z) l_0. \tag{27}$$

Similarly, for $\hbar$ small enough, we can have a uniform upper bound of α_z from equ.(25):

$$\exists\ a \text{ s.t. } \forall z, \alpha_z < a\hbar.$$

Equation (27) is correct only on a small distance l_0, but can be extend on a larger one d', by cutting it into N small intervals of length l_0, as shown on fig.(4). The property that the quantum flow is an isometry in $\mathcal{P}$ means that the distance between two different points is conserved. We deduce that the distance d_N between the state $[\psi(t)]$ and $[R(t),r(t)]$ is less than

$$d_N < N\ 2\tan(a\hbar)\ l_0.$$

Because $N = d'/l_0 \leq Cte\,/\sqrt{\hbar}$ for $\hbar \to 0$, we obtain $d_N < 2\,Cte\ l_0 \tan(a\hbar)/\sqrt{\hbar}$. We have $d = d_N \leq O(\sqrt{\hbar})$, as expected.

As a final remark, the expression equ.(24) depends on the complex coordinates (R,r) we have chosen on $\mathcal{S}$. But we could have expressed α using only objects from complex geometry, independent of the coordinates, as the metric g, the function $\mathcal{H}$, and Dolbeault operators [14][16] $\partial, \bar{\partial}$. We don't present them here because the result is not so illuminating.

5 Numerical illustration

In this section, the preceding results will be illustrated numerically on a specific model defined by the following Hamiltonian

$$\mathcal{H}(q,p) = -\cos(2\pi q) - \frac{1}{2}\cos(2\pi p) \qquad (28)$$

This is a one degree of freedom Hamiltonian. Trajectories are shown on fig.5 (a).

This Hamiltonian is known as the Harper model, and can be seen as a Hamiltonian on the toroidal phase space $(q,p) \in [0,1[^2$[9].

Let N be the number of planck cells on this torus. So $N = 1/h$. The semiclassical limit is obtained when $N \to \infty$.

From equ.(21) we calculate $\alpha(q,p)$ which represents the angle by which a coherent state located in (q,p) leaves the surface $\mathcal{S}$, during its early evolution. The function $\alpha(q,p)$ is represented on fig.5 (b). $\alpha(q,p)$ expresses also the amplitude of the deformation of the Husimi distribution of $|q,p>$ during its early evolution. Its is therefore natural to observe strong values of α at S_1 and S_2.

We consider now the evolution of a coherent state $|\psi(0)>=|qp>$ which is located on point A of fig.5 (b) at time $t=0$. On fig.6 (a) we can observe the Husimi distribution of the exact quantum state $|\psi(t)>$ on a period $T = 0.284$. (For a given state $|\psi>$, the Husimi distribution is the positive function $h_\psi(q,p) = |<qp|\psi>|^2$ on phase space, which informs directly on the density probability on phase space [18].)

This evolution is approximately described by the squeezed coherent states $|R(t)\ r(t)>$. The equation of motion for $r(t)R(t)$ are obtained by the projection procedure explained in the preceding section. They coincide with the evolution equations given in [17] by Heller. Figure 6 (b) shows the Husimi distribution of these states $|R(t)r(t)>$. The mean displacement of the distribution on phase space is described by $z(t) = r(t) - R(t)\bar{z}(t)$ while $R(t)$ describes the squeezing of the distribution. The same evolution of $z(t)$ is obtained, without squeezing when the quantum trajectory is projected of the surface $\mathcal{S}$ of standard coherent states. The Husimi distribution (not shown) would be a circular distribution following the classical point.

The disagreement between the exact evolution (a) and the approximate evolution with squeezed states (b) appears quickly, and corresponds to non elliptical deformations.

More quantitatively, fig.7 represents the Fubiny Study distance $d(t)$, calculated from equ.(1), between the exact quantum evolution $|\psi(t)>$ and the approximate standard coherent state $|z(t)>$, and also between $|\psi(t)>$ and the squeezed coherent state $|R(t)\ r(t)>$. We clearly observe that the latter approximation is better, for short time. More precisely, at $t=0$, these curves $d(t)$, have a derivative which is proportional to $\alpha/\sqrt{\hbar}$, where α is the angle of fig.(1). For $\hbar \to 0$, this angle goes to zero for squeezed coherent states, and tends to a constant value for the standard coherent states.

Finally, fig.(8) shows the distance d between the exact evolution and its approximation by a coherent state (standard or squeezed), after a fixed duration $t = T/4$, and for different values of $N = 1/h$. One clearly observes that for standard coherent states, this distance converges to a non zero constant for $\hbar \to 0$, as expected by equ.(22); this is because the deformation is not included. On the contrary in the approximation by a squeezed coherent state, this distance seems to converge to zero, as expected by equ.(26).

6 Conclusion

We have given a geometrical presentation of the semi-classical limit in the projective space. Essentially, we have shown that the orthogonal projection of the quantum velocity vector on the manifold of coherent states defines a Hamiltonian dynamic. This formulation is equivalent to the time-dependent-variational-principle. In this geometrical presentation, we have shown that a quantum trajectory leaves the manifold of standard coherent states with an angle of order $\sqrt{\hbar}$. Therefore, this trajectory becomes tangent to the manifold in the semi-classical limit $\hbar \to 0$.

If we enlarge the family of coherent states to the squeezed coherent states, we have shown that the angle diminishes to order $\hbar$, with a better description of the quantum dynamics. This improvement could be pursued by considering an enlarged family, generalizing equ.(11) and equ.(23) by:

$$|r, R, f>= \exp(\frac{R}{2}a^{+2} + ra^{+})(1 + fa^{+3})|0> .$$

$R \in \mathbb{C}$ describes elliptical fluctuations of the wave packet, and $f \in \mathbb{C}$ describes fluctuations of order 3. By a similar calculation, it can be shown that the quantum trajectory leaves this family with an angle of order $\hbar^{3/2}$, if $f = 0$.

When applied to the spin coherent states [19], constructed from the $SU(2)$ group in the irreducible representation j, it can be shown that the angle is of order $\alpha \sim 1/\sqrt{j}$ in the classical limit $j \to \infty$.

The calculation of this angle could be done more generally for different families of states where the variational principle is used, such as Slater determinants, Fermions in the Hartree Fock Bogoliubov approximation, other generalized coherent states [19], or even within mixed models like spin boson models. As we have remarked, this angle gives valuable informations on the validity of the approximation.

For longer times $t \gg 1$, the wave packet is spreading and can have auto-interference effects. The local description with a family of coherent states is then inefficient. On the contrary, a semi-classical description with the Van-Vleck formula (obtained using the stationary phase approximation in the Feynman path integral) [6] is then more appropriate. But it necessitates many classical trajectories and this approximation can not be described by a specific parametrized family of states (as coherent states for example).

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List of Figures