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The Ehrenfest picture and the geometry of Quantum Mechanics

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Summary. — In this paper we develop a picture of Quantum Mechanics based on the description of physical observables in terms of expectation value functions, generalizing thus the so called Ehrenfest theorems for quantum dynamics. Our basic technical ingredient is the set of tools which has been developed in the last years for the geometrical formulation of Quantum Mechanics. In the new picture, we analyze the problem of the dynamical equations, the uncertainty relations and interference and illustrate the construction with the simple case of a two-level system.

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1. – Introduction

The paradigmatic example of matter waves (see [1]), *e.g.*, electron interference, shows very neatly that we have at least three important aspects of quantum systems:

- a wave-like behavior incorporated in the Schrödinger picture;
- a corpuscular-like behavior at the detector giving rise to the Heisenberg picture;
- and a probabilistic-statistical behavior which emerges from the erratic behavior of the clicking of the detectors.

A closer scrutiny of this last aspect suggests that a good approach to the description of a quantum system would be to formulate Quantum Mechanics in terms of expectation value functions.

Let us assume that we have multiple copies of a given quantum system and let us consider the experiment in which we measure the position of the detector which clicks. After a sufficient long time, we would end up with a set of values in the form

$$e_Q(\psi) = \frac{\langle\psi|\hat{Q}|\psi\rangle}{\langle\psi|\psi\rangle}\,, \tag{1}$$

where $|\psi\rangle$ represents in the Dirac bra-ket notation the vectors of a Hilbert space $\mathcal{H}$ and $\hat{Q}$ represents the position operator acting on $\mathcal{H}$. More generally, if we perform measurements of other observable, say $\hat{A}$, we would obtain

$$e_A(\psi) = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}\,. \tag{2}$$

Thus the probabilistic-statistical aspect of Quantum Mechanics is captured by elaborating a picture completely given in terms of expectation value functions. Historically, expectation value functions appear already in the so-called *Ehrenfest theorem* (see [2]). In this work, we ellaborate on it to define an alternative picture of Quantum Mechanics.

We will argue that expectation value functions are able to provide an alternative picture of Quantum Mechanics with respect to the Schrödinger or the Heisenberg ones. For instance, for a system described by a Hamiltonian operator in the form

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \hat{V}(x),$$

we would obtain a dynamical system at the level of the expectation value functions as

$$\frac{\mathrm{d}}{\mathrm{d}t}e_Q(\psi) = \frac{1}{m}e_P(\psi); \qquad \frac{\mathrm{d}}{\mathrm{d}t}e_Q(\psi) = -e_{\mathrm{grad}\,V}(\psi); \tag{3}$$

which is usually known as the Ehrenfest theorem. It is appropriate to remark that already Koopman [3] and von Neuman [4] proved that both Classical and Quantum Mechanics can be treated in this picture. We recall that while Quantum Mechanics would be formulated on the Hilbert space of square-integrable complex-valued functions on the "configuration" or the "momentum" space to ensure the irreducibility of the representation of the Heisenberg-Weyl algebra; Classical Mechanics would be formulated on the Hilbert space of square-integrable complex-valued functions on the full phase-space.

2. – The tensors of the geometric formulation of Quantum Mechanics

The aim of this section is simply to provide a tensorial characterization of Quantum Mechanics. We shall see later how the tensors obtained now will provide us with the necessary tools for our definition of the Ehrenfest picture of Quantum Mechanics. The section contains a brief summary of the results presented in several recent works as [1, 5-8]. We also address the interested reader to some other references by serveral authors covering similar topics. Just to mention the most relevant references ordered chronologically, let us refer to former interesting approaches as [9], the seminal work by Kibble [10], the works by Cantoni [11-15], by Cirelli and co-workers [16, 17], the more physically oriented approach by Heslot [18], Bloch's paper [19], the work by Anandan [20,21], and then Ashtekar and Schilling [22]. There are several interesting works by Brody and coworkers, [23] being the one closer to the work presented here and also from Spera and coworkers [24, 25].

2·1. *Representation of pure states.* – The first step is to replace the Hilbert space $\mathcal{H}$ which models the set of vector states by a description in terms of real differential manifolds. Thus we replace the Hilbert space $\mathcal{H}$ with its realification $\mathcal{H}_{\mathbb{R}} := M_Q$. In this realification process the complex structure on $\mathcal{H}$ will be represented by a tensor J on M_Q as we will see. We assume that the dimension of the manifold M_Q is equal to $2n$.

The natural identification is then provided by choosing a basis $\{|z_k\rangle\}$ in $\mathcal{H}$ and splitting the corresponding coordinates into their real and imaginary parts:

$$|\psi\rangle = \sum_k \psi_k |z_k\rangle \qquad \psi_k \to \psi_k^R + i\psi_k^I.$$

Then,

$$\{\psi_1, \dots, \psi_n\} \in \mathcal{H} \mapsto \{\psi_1^R, \dots, \psi_n^R, \psi_1^I, \dots \psi_n^I\} \equiv (\Psi_R, \Psi_I) \in \mathcal{H}_{\mathbb{R}}.$$

Under this transformation, the Hermitian product becomes, for $\psi^1, \psi^2 \in \mathcal{H}$

$$\langle(\Psi_R^1, \Psi_I^1), (\Psi_R^2, \Psi_I^2)\rangle = (\langle\Psi_R^1, \Psi_R^2\rangle + \langle\Psi_I^1, \Psi_I^2\rangle) + i(\langle\Psi_R^1, \Psi_I^2\rangle - \langle\Psi_I^1, \Psi_R^2\rangle).$$

To consider $\mathcal{H}_{\mathbb{R}}$ just as a real differential manifold, the algebraic structures available on $\mathcal{H}$ must be converted into tensor fields on $\mathcal{H}_{\mathbb{R}}$. Consider first the tangent and cotangent bundles $T\mathcal{H}$ and $T^*\mathcal{H}$ and the following structures:

– The complex structure of $\mathcal{H}$ is translated into a tensor

$$J : M_Q \to M_Q,$$

satisfying $J(\Psi_R, \Psi_I) = (-\Psi_I, \Psi_R)$ for any point $(\Psi_R, \Psi_I) \in M_Q$. It is immediate to verify that in this case

$$J^2 = -\mathbb{I}.$$

– The linear structure available in M_Q is encoded in the vector field Δ

$$\Delta : M_Q \to TM_Q \qquad \psi \mapsto (\psi, \psi).$$

– With every vector we can associate a vector field

$$X_\psi : M_Q \to TM_Q \qquad \phi \to (\phi, \psi).$$

These vector fields are the infinitesimal generators of the vector group M_Q acting on itself.

– The Hermitian tensor $\langle \cdot, \cdot \rangle$ defined on the complex vector space $\mathcal{H}$, can be written in geometrical terms as

$$\langle X_{\psi_1}, X_{\psi_2} \rangle(\phi) = \langle \psi_1, \psi_2 \rangle.$$

On the "real manifold" the Hermitian scalar product may be written as

$$\langle \psi_1, \psi_2 \rangle = g(X_{\psi_1}, X_{\psi_2}) + i\,\omega(X_{\psi_1}, X_{\psi_2}),$$

where g is now a symmetric tensor and ω a skew-symmetric one.

The properties of the Hermitian product ensure that:

– the symmetric tensor is positive definite and non-degenerate, and hence defines a Riemannian structure on the real vector manifold.

– the skew-symmetric tensor is also non degenerate, and is closed with respect to the natural differential structure of the vector space. Hence, the tensor is a symplectic form (see also [26]).

As the inner product is sesquilinear, it satisfies

$$\langle \psi_1, i\psi_2 \rangle = i\langle \psi_1, \psi_2 \rangle, \qquad \langle i\psi_1, \psi_2 \rangle = -i\langle \psi_1, \psi_2 \rangle.$$

This implies

$$g(X_{\psi_1}, X_{\psi_2}) = \omega(JX_{\psi_1}, X_{\psi_2}).$$

We also have that $J^2 = -\mathbb{I}$, and hence that the triple (J, g, ω) defines a Kähler structure (see [16]). This implies, among other things, that the tensor J generates both finite and infinitesimal transformations which are orthogonal and symplectic.

The choice of the basis also allows us to introduce adapted coordinates for the realified structure:

$$\langle z_k, \psi \rangle = (q_k + ip_k)(\psi),$$

and write the geometrical structures introduced above as

$$J = \partial_{p_k} \otimes \mathrm{d}q_k - \partial_{q_k} \otimes \mathrm{d}p_k, \qquad g = \mathrm{d}q_k \otimes \mathrm{d}q_k + \mathrm{d}p_k \otimes \mathrm{d}p_k, \qquad \omega = \mathrm{d}q_k \wedge \mathrm{d}p_k.$$

Note 1. *If we represent the points of $\mathcal{H}$ by using complex coordinates we can write the Hermitian structure by means of $z_n = q^n + ip_n$:*

$$h = \sum_k \mathrm{d}\bar{z}_k \otimes \mathrm{d}z_k,$$

where of course

$$\langle X_{\psi_1} | X_{\psi_2} \rangle = h(X_{\psi_1}, X_{\psi_2}),$$

the vector fields now being the corresponding ones on the complex manifold.

In an analogous way we can consider a contravariant version of these tensors. The coordinate expressions with respect to the natural basis are

– the Riemannian structure

$$G = \sum_{k=1}^{n} \left(\frac{\partial}{\partial qk} \otimes \frac{\partial}{\partial q^k} + \frac{\partial}{\partial p_k} \otimes \frac{\partial}{\partial p_k} \right), \tag{4}$$

– the Poisson tensor

$$\Omega = \sum_{k=1}^{n} \left(\frac{\partial}{\partial q^k} \wedge \frac{\partial}{\partial p_k} \right), \tag{5}$$

– while the complex structure has the form

$$J = \sum_{k=1}^{n} \left(\frac{\partial}{\partial p_k} \otimes \mathrm{d}q^k - \frac{\partial}{\partial q^k} \otimes \mathrm{d}p_k \right). \tag{6}$$

2˙1.1. Example I: the Hilbert space of a two level quantum system. For a two levels system we will consider an orthonormal basis on $\mathbb{C}^2$, say $\{|e_1\rangle, |e_2\rangle\}$. We introduce thus a set of coordinates

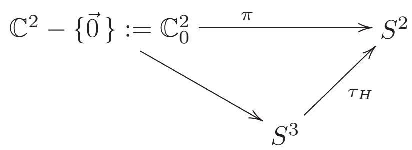
$$\langle e_j|\psi\rangle = z^j(\psi) = q^j(\psi) + ip_j(\psi) \qquad j = 1, 2.$$

In the following we will use z^j or q^j, p_j omitting the dependence in the state ψ as it is usually done in differential geometry.

The set of physical states is not equal to $\mathbb{C}^2$, since we have to consider the equivalence relation given by the multiplication by a complex number *i.e.*

$$\psi_1 \sim \psi_2 \Leftrightarrow \psi_2 = \lambda\psi_1 \qquad \lambda \in \mathbb{C}_0 = \mathbb{C} - \{0\}.$$

And besides, the norm of the state must be equal to one. These two properties can be encoded in the following diagram:



where S^2 and S^3 stand for the two and three dimensional spheres, and the projection τ_H defines the Hopf fibration. The projection π is associating each vector with the one-dimensional complex vector space to which it belongs. Thus we see how this projection factorizes through a projection onto S^3 and a further projection given by the Hopf fibration, which is a $U(1)$-fibration.

The Hermitian inner product on $\mathbb{C}^2$ can be written in the coordinates z_1, z_2 as

$$\langle\psi|\psi\rangle = \bar{z}_j z^k \langle e_k|e_j\rangle = \bar{z}_j z^j.$$

Equivalently we can write it in real coordinates q, p and obtain

$$\langle\psi|\psi\rangle = p_1^2 + p_2^2 + (q^1)^2 + (q^2)^2.$$

We can also obtain these tensors in contravariant form if we take as starting point the Hilbert space $\mathcal{H} = \mathbb{C}^2$. If we repeat the steps above, we obtain the two contravariant tensors:

$$G = \frac{\partial}{\partial q^1}\otimes\frac{\partial}{\partial q^1} + \frac{\partial}{\partial p_1}\otimes\frac{\partial}{\partial p_1} + \frac{\partial}{\partial q^2}\otimes\frac{\partial}{\partial q^2} + \frac{\partial}{\partial p_2}\otimes\frac{\partial}{\partial p_2}\,; \qquad \Omega = \frac{\partial}{\partial q^1}\wedge\frac{\partial}{\partial p_1} + \frac{\partial}{\partial q^2}\wedge\frac{\partial}{\partial p_2}\,.$$

Other tensors encode the complex vector space structure of $\mathcal{H} = \mathbb{C}^2$:

– the dilation vector field $\Delta = q^1\frac{\partial}{\partial q^1} + p_1\frac{\partial}{\partial p_1} + q^2\frac{\partial}{\partial q^2} + p_2\frac{\partial}{\partial p_2}$,

– and the complex structure tensor $J = \mathrm{d}p_1\otimes\frac{\partial}{\partial q^1} - \mathrm{d}q^1\otimes\frac{\partial}{\partial p_1} + \mathrm{d}p_2\otimes\frac{\partial}{\partial q^2} - \mathrm{d}q^2\otimes\frac{\partial}{\partial p_2}$.

By combining both tensors, we can define the infinitesimal generator of the multiplication by a phase:

$$\Gamma = J(\Delta) = p_1\frac{\partial}{\partial q^1} - q^1\frac{\partial}{\partial p^1} + p_2\frac{\partial}{\partial q^2} - q^2\frac{\partial}{\partial p^2}\,.$$

Thus we see how Δ is responsible for the quotienting from $\mathbb{C}_0^2$ onto S^3, while Γ is responsible for the Hopf fibration $S^3 \to S^2$.

2˙2. *The complex projective space*. – In the formulation as a real vector space, we can represent the multiplication by a phase on the manifold M_Q as a transformation whose infinitesimal generator is written as

$$\Gamma = \sum_k \left(p_k\frac{\partial}{\partial q^k} - q^k\frac{\partial}{\partial p_k}\right). \tag{7}$$

We can also consider another important vector field, which encodes the linear space structure of the tangent bundle TM_Q. In order to avoid singularities let us eliminate the zero section of the bundle TM_Q and denote the resulting space by T_0M_Q. We remind the reader that M_Q is just the realification of a complex vector space and, as such, we can encode its linear structure in the dilation vector field, which reads

$$\Delta : M_Q \to T_0M_Q; \qquad \psi \mapsto (\psi, \psi). \tag{8}$$

In the coordinate system (q^k, p_j), it takes the form

$$\Delta = q^k\frac{\partial}{\partial q^k} + p_k\frac{\partial}{\partial p_k}\,. \tag{9}$$

We are particularly interested in the relation of the vector fields Δ and Γ. In particular:

Lemma 1. Δ *and* Γ *define a foliation on the manifold* M_Q.

Proof. It is simple to relate Δ with Γ via the complex structure, in the form

$$\Gamma = J(\Delta). \tag{10}$$

Then it is straightforward to prove that both vector fields commute. □

We thus have an integrable distribution defined on the manifold M_Q. We can thus define the corresponding quotient manifold identifying the points which belong to the same orbit of the generators Γ and Δ. Notice that, from the physical point of view, this corresponds to the identification of points in the same ray of the Hilbert space.

Definition 1. *The resulting quotient manifold, denoted as $\mathcal{P}$, defined as*

$$\pi : M_Q \to \mathcal{P} \tag{11}$$

is the complex projective space and its points represent the physical pure states of a quantum system. We will denote by $[\psi]$ the point in $\mathcal{P}$ which is the image by π of a point $\psi \in M_Q$:

$$\mathcal{P} \ni [\psi] := \pi(\psi) \qquad \psi \in M_Q. \tag{12}$$

3. – The Ehrenfest picture for pure states

Having introduced the necessary tools, let us proceed to describe the Ehrenfest picture of Quantum Mechanics. As we saw in the introduction, the key point consists in the description of physical observables in terms of expectation value functions. If we accept the point of view of formulating Quantum Mechanics in terms of expectation value functions, we must also accept that they are not defined on $\mathcal{H}$ but rather they are functions on the arguments $\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$. This means that they are really functions defined on the Hilbert space $\mathcal{H}$ (or M_Q) which represent functions on the projective space $\mathcal{P}$ corresponding to $\mathcal{H}$. This change in the carrier space is not without consequences because now the carrier space is not linear anymore: instead of a Hilbert space we must consider a Hilbert manifold. This implies that we have to face the problems of describing interference, superpositions of states and the composition of expectation value functions to replace the multiplication rule of operators.

Therefore, we must consider functions on M_Q which are constant along the fibers of the fibration $\pi : M_Q \to \mathcal{P}$. Thus functions, meaningful from a physical point of view, correspond to

$$e_A(\psi) = \frac{\langle\psi|A\psi\rangle}{\langle\psi|\psi\rangle}\,. \tag{13}$$

These are functions on M_Q which are in one-to-one correspondence with the functions on the projective space $\mathcal{P}$ as pullback via the projection defined in eq. (11). Obviously, they are no longer quadratic; but this is a natural property taking into account that the projective space $\mathcal{P}$ has lost the linear structure of M_Q to become just a differential manifold.

3˙1. *The spectral information.* – One of the main aspects we must recover from the usual picture is the spectrum of the operators. Indeed, in the usual descriptions of Quantum Mechanics the spectrum of the observables encodes most of the information associated to the corresponding physical quantity. Thus, in the Hilbert space description, given the observable $\hat{A}$, we associate with it the basis of eigenvectors $\{|v_a\rangle\}$ and the corresponding eigenvalues:

$$\hat{A}|v_a\rangle = a|v_a\rangle.$$

Given a system in a state $|\psi(t)\rangle$, we also know that the probability for a measurement of the observable $\hat{A}$ at time t to give the result a is given by

$$\mathcal{P}_a = |\langle v_a|\psi(t)\rangle|^2.$$

How can we recover this information by using the expectation value function e_A defined by eq. (2)? Notice that we are considering it as a function defined the space of states M_Q obtained by realification of the Hilbert space $\mathcal{H}$. In this context, the information about the spectrum is recovered easily from the set of critical points of the function. Indeed, it is immediate to prove that the function e_A has a critical point at each eigenvector $|v_a\rangle$ while the value that it takes at those points of M_Q is precisely the eigenvalue of the operator $\hat{A}$:

$$\hat{A}|v_a\rangle = a|v_a\rangle \Leftrightarrow \begin{cases} de_A(|v_a\rangle) = 0, \\ e_A(|v_a\rangle) = a. \end{cases} \tag{14}$$

3˙2. *The dynamics and the Poisson tensor.* – We can also study the evolution of the system in the new picture. Let us consider a pure state

$$\rho_\psi(t) = \frac{|\psi(t)\rangle\langle\psi(t)|}{\langle\psi(t)|\psi(t)\rangle} \tag{15}$$

and assume that the evolution is ruled by a one-parameter group of transformations associated with a one-parameter group of unitary transformations of the Hilbert space $\mathcal{H}$. At the level of the function e_A we can write

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{\langle\psi(t)|\psi(t)} \left[\left\langle \frac{\mathrm{d}\psi(t)}{\mathrm{d}t}\middle|\hat{A}\psi(t)\right\rangle + \left\langle \psi(t)\middle|\hat{A}\frac{\mathrm{d}\psi(t)}{\mathrm{d}t}\right\rangle\right], \tag{16}$$

where we assume that the evolution preserves the norm of the state $|\psi(t)\rangle$ and that $\hat{A}$ does not depend explicitely on time.

From Stone's theorem, we know that the unitary evolution on the Hilbert space $\mathcal{H}$ is generated by a skew-Hermitian generator in the form

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{17}$$

for some Hermitian operator $\hat{H}$. If we introduce the commutator of the operators $\hat{H}$ and $\hat{A}$ as

$$[\hat{H},\hat{A}] = i(\hat{H}\hat{A} - \hat{A}\hat{H}), \tag{18}$$

eq. (16) can be written in terms of expectation value functions as

$$i\frac{\mathrm{d}}{\mathrm{d}t}e_A(\psi) = -\frac{\langle\psi|\hat{H}\hat{A} - \hat{A}\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = ie_{[\hat{H},\hat{A}]}(\psi). \tag{19}$$

If we want to formulate completely the problem in terms of expectation value functions, it makes sense to introduce an operation on this set of functions, in particular a *quantum Poisson bracket* defined as

$$\{e_H, e_A\} := e_{[\hat{H},\hat{A}]}. \tag{20}$$

We can extend this construction to the space of expectation value functions by defining a bidifferential operator $\Omega_{\mathcal{P}}$ which represents the Poisson tensor corresponding to the bracket above:

$$\Omega_{\mathcal{P}}(\mathrm{d}e_A, \mathrm{d}e_B) := \{e_A, e_B\}. \tag{21}$$

Notice that these tensors, even if they are defined on the manifold M_Q, are not the same as the tensor in eq. (5). Indeed, the functions are projectable under $\pi : M_Q \to \mathcal{P}$, but it is simple to understand that the product under (G and) Ω is not, since the tensors are of degree -2, *i.e.*, the Lie derivative of the tensors with respect to the dilation vector field Δ defined in eq. (8) is

$$\mathcal{L}_\Delta \Omega = -2\Omega.$$

Thus, in order to make it projectable, we must rescale it by a factor of degree two, as for instance the square of norm of $|\psi\rangle$ which is a central element:

$$\{e_A, e_B\}_{\mathcal{P}} := \Omega_{\mathcal{P}}(\mathrm{d}e_A, \mathrm{d}e_B) = \langle\psi|\psi\rangle\{e_A, e_B\}. \tag{22}$$

3·3. *Indetermination relations and the symmetric structure.* – Another aspect that we have to take into account in our description is the formulation in terms of expectation value funtions of another important aspect of Quantum Mechanics as it is the indetermination relations. This introduces the necessity of bringing the tensor $G_{\mathcal{P}}$, defined in a similar way as we did for $\Omega_{\mathcal{P}}$, into play.

It is simple to verify that, given an operator $\hat{A}$, its squared uncertainty (its variance) can be obtained from the expectation value function e_A as

$$(\Delta A)^2 = \langle \mathrm{d}e_A|\mathrm{d}e_A\rangle = e_{A^2} - (e_A)^2, \tag{23}$$

where we represent by d the exterior differential in $\mathcal{H}$ and we use the extension of the Hermitian structure to the differential one-forms.

But if we want to implement the variance directly at the level of the projective space $\mathcal{P}$, we need to introduce a differential operator which encodes the symmetric product of operators at the level of the expectation value functions. We consider then the corresponding tensor which precisely coincides with the tensor $G_{\mathcal{P}}$:

$$G_{\mathcal{P}}(\mathrm{d}e_A, \mathrm{d}e_B) := e_{AB+BA} - e_A e_B. \tag{24}$$

This symmetric tensor $G_{\mathcal{P}}$ together with the tensor $\Omega_{\mathcal{P}}$ defined in eq. (21) endow the projective space with a Hermitian bidifferential operator. We shall work explicitly the various aspects of the construction by means of a very simple example: a two level system defined on a Hilbert space $\mathcal{H} = \mathbb{C}^2$.

3˙3.1. Example II: the projective space for a two-level quantum system. Extending the example presented in sect. **2**˙1.1, we can consider now the corresponding projective space and the corresponding tensors. It is important to remark that while forms can not be projected, contravariant tensor fields can. This is the reason why we introduced the contravariant tensors Λ and G. Thus by considering

$$G = \frac{\partial}{\partial q^1} \otimes \frac{\partial}{\partial q^1} + \frac{\partial}{\partial p_1} \otimes \frac{\partial}{\partial p_1} + \frac{\partial}{\partial q^2} \otimes \frac{\partial}{\partial q^2} + \frac{\partial}{\partial p_2} \otimes \frac{\partial}{\partial p_2},$$

we can consider the projection of the tensor. As it happens with the Poisson tensor, it is immediate to understand that such a tensor can not be projected directly, since it is of degree two with respect to the dilations, *i.e.*

$$\mathcal{L}_\Delta G = -2G.$$

Therefore, we have to consider a conformal factor and define (see [27]):

$$\begin{aligned} G_{\mathcal{P}} = {} & \langle\psi|\psi\rangle G - \Gamma \otimes \Gamma - \Delta \otimes \Delta = \\ & \left((q^1)^2 + (q^2)^2 + p_1^2 + p_2^2\right) \\ & \times \left(\frac{\partial}{\partial q^1} \otimes \frac{\partial}{\partial q^1} + \frac{\partial}{\partial p_1} \otimes \frac{\partial}{\partial p_1} + \frac{\partial}{\partial q^2} \otimes \frac{\partial}{\partial q^2} + \frac{\partial}{\partial p_2} \otimes \frac{\partial}{\partial p_2} \right) \\ & - \sum_{lm} \left(p_l \frac{\partial}{\partial q^l} - q^l \frac{\partial}{\partial p_l} \right) \otimes \left(p_m \frac{\partial}{\partial q^m} - q^m \frac{\partial}{\partial p_m} \right) \\ & - \sum_{lm} \left(q^l q^m \frac{\partial}{\partial q^l} \otimes \frac{\partial}{\partial q^m} + p_l p_m \frac{\partial}{\partial p_l} \otimes \frac{\partial}{\partial p_m} \right). \end{aligned} \tag{25}$$

Analogously we can write the coordinate expression of the tensor $\Omega_{\mathcal{P}}$:

$$\begin{aligned} \Omega_{\mathcal{P}} = {} & \langle\psi|\psi\rangle \Omega - \Gamma \otimes \Delta - \Delta \otimes \Gamma = \\ & \left((q^1)^2 + (q^2)^2 + p_1^2 + p_2^2\right) \left(\frac{\partial}{\partial q^1} \wedge \frac{\partial}{\partial p^1} + \frac{\partial}{\partial q^2} \wedge \frac{\partial}{\partial p^2} \right) \\ & - \sum_{lm} \left(p_l \frac{\partial}{\partial p_l} + q^l \frac{\partial}{\partial q^l} \right) \otimes \left(p_m \frac{\partial}{\partial q^m} - q^m \frac{\partial}{\partial p_m} \right) \\ & - \sum_{lm} \left(p_l \frac{\partial}{\partial q^l} - q^l \frac{\partial}{\partial p_l} \right) \otimes \left(p_l \frac{\partial}{\partial p_l} + q^l \frac{\partial}{\partial q^l} \right). \end{aligned} \tag{26}$$

3˙4. *Uncertainty relations*. – From the definition of the variance, we can write the Robertson version of the uncetainty relations (see [28]) in a simple form:

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{4} \langle\psi|[A, B]\psi\rangle^2. \tag{27}$$

We are going to obtain this well known expression within our Ehrenfest picture. Let us consider an arbitrary operator F on $\mathcal{H}$. It is immediate that

$$\langle\psi|F^\dagger F\psi\rangle \geq 0; \qquad \forall\,|\psi\rangle \in \mathcal{H}.$$

For simplicity, we will restrict the set of states to the sphere of normalized states $\mathcal{S}$, *i.e.* we shall consider the inequality

$$\langle\psi|F^\dagger F\psi\rangle \geq 0; \qquad \forall\,|\psi\rangle \in \mathcal{S}. \tag{28}$$

Let us choose F to be the operator which is a complex linear combination of two Hermitian observables:

$$F = (A - \langle A\rangle_\psi \mathbb{I}) + i\alpha(B - \langle B\rangle_\psi \mathbb{I}), \qquad \alpha \in \mathbb{R}, \tag{29}$$

where $\langle A\rangle_\psi$ and $\langle B\rangle_\psi$ represent the expectation value of each observable in a given state.

In this situation, the inequality (28), as a polynomial in α, corresponds to

$$\alpha^2 \left(e_{B^2}(\psi) - e_B(\psi)^2\right) + \alpha e_{[A,B]}(\psi) + \left(e_{A^2}(\psi) - e_A(\psi)^2\right) \geq 0, \tag{30}$$

where $[A,B] = i(AB - BA)$ to make it an inner operation in the set of Hermitian operators.

The condition must hold for any value of α and hence we obtain a condition on the roots, that can not be real. Then, we obtain

$$4\left(e_{B^2}(\psi) - e_B(\psi)^2\right)\left(e_{A^2}(\psi) - e_A(\psi)^2\right) - e_{[A,B]}(\psi)^2 \geq 0 \tag{31}$$

or, equivalently,

$$\left(e_{B^2}(\psi) - e_B(\psi)^2\right)\left(e_{A^2}(\psi) - e_A(\psi)^2\right) \geq \frac{1}{4} e_{[A,B]}(\psi)^2. \tag{32}$$

In this expression we recognize the usual formulation of the uncertainty relation for two arbitrary operators if we write

$$(\Delta A)_\psi = \left(e_{A^2}(\psi) - e_A(\psi)^2\right) \tag{33}$$

in this language, the relation becomes

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{4} e_{[A,B]}(\psi)^2. \tag{34}$$

This new expression allows us to write uncertainty relations by using only tensors $G_\mathcal{P}$ and $\Omega_\mathcal{P}$:

$$G_\mathcal{P}(\mathrm{d}e_A, \mathrm{d}e_A) G_\mathcal{P}(\mathrm{d}e_B, \mathrm{d}e_B) \geq \frac{1}{4}\left(\Omega_\mathcal{P}(\mathrm{d}e_A, \mathrm{d}e_B)\right)^2. \tag{35}$$

It is also possible to provide an analogous formulation for Schrödinger uncertainty relations (see [29]). Consider the same Hermitian operators A and B as above, and consider the expectation value of the product

$$K = K_A K_B = (A - \langle A \rangle_\psi \mathbb{I})(B - \langle B \rangle_\psi \mathbb{I}),$$

where $K_A = (A - \langle A \rangle_\psi \mathbb{I})$ and $K_B = (B - \langle B \rangle_\psi \mathbb{I})$. From Schwartz inequality, we can write

$$|\langle \psi | K \psi \rangle|^2 = |\langle \psi | K_A K_B | \psi \rangle|^2 \leq \langle \psi | K_A^2 | \psi \rangle \langle \psi | K_B^2 | \psi \rangle. \tag{36}$$

Now, we can replace the product $K_A K_B$ by

$$K_A K_B = \frac{1}{2}(K_A K_B + K_B K_A) + \frac{1}{2}(K_A K_B - K_B K_A) = \frac{1}{2}(K_A K_B + K_B K_A) + \frac{i}{2}[K_A, K_B].$$

We can write then

$$|\langle \psi | K_A K_B \psi \rangle|^2 = \frac{1}{4}\left(\langle | \psi (K_A K_B + K_B K_A) | \psi \rangle\right)^2 + \frac{1}{4}(\langle \psi | [K_A, K_B] \psi \rangle)^2.$$

It is straightforward to verify that

$$\langle \psi | [K_A, K_B] \psi \rangle = \langle \psi | [A, B] | \psi \rangle,$$

because the identity operators trivially commute; and

$$\langle \psi | (K_A K_B + K_B K_A) | \psi \rangle = \langle \psi | (AB + BA) | \psi \rangle - \langle \psi | A \psi \rangle \langle \psi | B | \psi \rangle.$$

Analogously

$$\langle \psi | K_A^2 | \psi \rangle = \langle \psi | A^2 | \psi \rangle - \langle \psi | A | \psi \rangle^2; \qquad K_B^2 | \psi \rangle = \langle \psi | B^2 | \psi \rangle - \langle \psi | B | \psi \rangle^2.$$

We can then write eq. (36) as

$$\begin{aligned} &(\langle \psi | A^2 | \psi \rangle - \langle \psi | A | \psi \rangle^2)(\langle \psi | B^2 | \psi \rangle - \langle \psi | B | \psi \rangle^2) \geq \\ &\frac{1}{4}\left(\langle \psi | (AB + BA) | \psi \rangle - \langle \psi | A \psi \rangle \langle \psi | B | \psi \rangle\right)^2 + \frac{1}{4}\langle \psi | [A, B] | \psi \rangle^2 \end{aligned} \tag{37}$$

or, analogously,

$$\begin{aligned} &(e_{A^2}(\psi) - e_A(\psi)^2)(e_{B^2}(\psi) - e_B(\psi)^2) \\ &\quad - \frac{1}{4}(e_{(A \circ B)}(\psi) - e_A(\psi) e_B(\psi))^2 \geq \frac{1}{4}\langle \psi | [A, B] | \psi \rangle^2, \end{aligned} \tag{38}$$

where $A \circ B = (AB + BA)$.

This expression, which is known as Schrödinger uncertainty relation, can also be written in terms of the tensors $G_\mathcal{P}$ and $\Omega_\mathcal{P}$ in the form

$$G_\mathcal{P}(\mathrm{d}e_A, \mathrm{d}e_A) G_\mathcal{P}(\mathrm{d}e_B, \mathrm{d}e_B) - \frac{1}{4} G_\mathcal{P}(\mathrm{d}e_A, \mathrm{d}e_B)^2 \geq \frac{1}{4}\Omega_\mathcal{P}(\mathrm{d}e_A, \mathrm{d}e_B). \tag{39}$$

4. – Ehrenfest picture for mixed states: the two levels system

In the previous section we have been able to construct, by using the tensors which encode the Hermitian structure of the Hilbert space of states, a formulation of Quantum Mechanics where the physical observables are represented by the expectation value functions associated to pure states of the physical system. The next step is to consider the generalization to the case of mixed states. For the sake of simplicity, we shall consider only the case of the two level system that we have analyzed so far. In order to do that, we shall begin by reformulating the construction above in terms of rank-one projectors, and later we will be able to extend this new framework to include arbitrary mixed states.

4˙1. *Reformulation of pure states.* – We know that the rank-one projectors defined on $\mathcal{H}$ are in one-to-one correspondence with the points of the projective space $\mathcal{P}$. Indeed, we can write

$$\begin{pmatrix} \bar{z}_1 z_1 & \bar{z}_1 z_2 \\ \bar{z}_2 z_1 & \bar{z}_2 z_2 \end{pmatrix} = \rho_\psi = y_0\sigma_0 + y_1\sigma_1 + y_2\sigma_2 + y_3\sigma_3, \tag{40}$$

where we have to impose that

$$\mathrm{Tr}\,\rho_\psi = 1 \Rightarrow y_0 = \frac{1}{2}$$

and

$$\mathrm{Tr}\,\rho_\psi^2 = \mathrm{Tr}\,\rho_\psi \Rightarrow y_0^2 + y_1^2 + y_2^2 + y_3^2 = \frac{1}{2} \Rightarrow y_1^2 + y_2^2 + y_3^2 = \frac{1}{4}.$$

We conclude thus that the set of rank-one projectors on vectors of the Hilbert space $\mathcal{H} = \mathbb{C}^2$, which is in one-to-one correspondence with the points of the projective space $\mathcal{P} = \mathbb{CP}^1$ is diffeomorphic to the two-dimensional sphere S^2.

The coordinates $\{y_0, y_1, y_2, y_3\}$ can be obtained from the properties of the Pauli matrices:

$$y_0 = \frac{1}{2}\,\mathrm{Tr}(\sigma_0\rho_\psi) = \frac{1}{2}$$

and

$$y_j = \frac{1}{2}\,\mathrm{Tr}(\sigma_j\rho_\psi).$$

Expectation value functions can be defined for any Hermitian operator in the form

$$A = a_0\sigma_0 + \alpha_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3,$$

as the evaluation of the operator on the state ρ:

$$\begin{aligned} e_A(\rho) &= \mathrm{Tr}(A\rho) = \mathrm{Tr}\left[A\left(\frac{1}{2}\sigma_0 + y_1\sigma_1 + y_2\sigma_2 + y_3\sigma_3\right)\right] \\ &= a_0 + 2(a_1y_1 + a_2y_2 + a_3y_3). \end{aligned} \tag{41}$$

The embedding of the set of pure states in this form, forces us to use Lagrange multipliers in order to, for instance, determine the set of critical points of the function $e_A(\rho)$ on the set of pure states. Thus, we compute the extremal points of the function

$$f_A(\lambda, \rho) = e_A(\rho) - \lambda \left(y_1^2 + y_2^2 + y_3^2 - \frac{1}{4} \right).$$

We obtain thus

$$\mathrm{d}f_A(y^\star) = 0 \to \begin{cases} 2[(a_1 - \lambda y_1^\star)\mathrm{d}y_1 + (a_2 - \lambda y_2^\star)\mathrm{d}y_2 + (a_3 - \lambda y_3^\star)\mathrm{d}y_3] = 0, \\ (y_1^\star)^2 + (y_2^\star)^2 + (y_3^\star)^2 - \frac{1}{4} = 0. \end{cases}$$

This implies that

$$y_1^\star = \frac{a_1}{\lambda}; \qquad y_2^\star = \frac{a_2}{\lambda}; \qquad y_3^\star = \frac{a_3}{\lambda}$$

and thus

$$a_1^2 + a_2^2 + a_3^2 = \frac{1}{4}\lambda^2 \Rightarrow \lambda = \pm\sqrt{4(a_1^2 + a_2^2 + a_3^2)}.$$

The corresponding eigenvalue is obtained as

$$e_A(\rho^\star) = a_0 \pm \frac{2}{\sqrt{4(a_1^2 + a_2^2 + a_3^2)}} \left(a_1^2 + a_2^2 + a_3^2\right) = a_0 \pm \sqrt{(a_1^2 + a_2^2 + a_3^2)}. \tag{42}$$

If we consider a second operator

$$B = b_0\sigma_0 + b_1\sigma_1 + b_2\sigma_2 + b_3\sigma_3 \tag{43}$$

and the corresponding function $e_B(\rho)$, we can evaluate the commutator and the skew-commutator:

$$[A, B] := i(AB - BA), \tag{44}$$
$$A \circ B = (AB + BA), \tag{45}$$

and the corresponding functions:

$$e_{[A,B]}(\rho) = 4(a_3b_2 - a_2b_3)y_1 + 4(a_1b_3 - a_3b_1)y_2 + 4(a_2b_1 - a_1b_2)y_3; \tag{46}$$

and

$$\begin{aligned} e_{A\circ B}(\rho) = {} & 4(a_0b_0 + a_1b_1 + a_2b_2 + a_3b_3)y_0 + 4(a_1b_0 + a_0b_1)y_1 \\ & +4(a_2b_0 + a_0b_2)y_2 + 4(a_3b_0 + a_0b_3)y_3. \end{aligned} \tag{47}$$

From both expressions we read therefore the coordinate expression of the tensors representing the operations at the level of the expectation value functions:

$$G(\rho) = 4\left(y_0 \sum_{j=0}^{4} \frac{\partial}{\partial y_j} \otimes \frac{\partial}{\partial y_j} + \sum_{j=1}^{3}\left(y_j \frac{\partial}{\partial y_j} \otimes \frac{\partial}{\partial y_0} + y_j \frac{\partial}{\partial y_0} \otimes \frac{\partial}{\partial y_j}\right)\right), \tag{48}$$

$$\Lambda(\rho) = \sum_{jkl=1}^{3} \epsilon^{jkl} y_j \frac{\partial}{\partial y_k} \wedge \frac{\partial}{\partial y_l}. \tag{49}$$

4˙2. *Ehrenfest picture of mixed states.* – The set of mixed states $\mathcal{D}$ can be defined by relaxing the condition defining the projector property of ρ, *i.e.*,

$$\mathcal{D} = \{\rho \in \mathfrak{u}^*(\mathcal{H}) \mid \operatorname{Tr}\rho = 1\}. \tag{50}$$

By using the same coordinates, we end up with the following coordinate description:

$$\mathcal{D} = \left\{(y_1, y_2, y_3) \in \mathbb{R}^3 \mid y_1^2 + y_2^2 + y_3^2 \leq \frac{3}{4}\right\}. \tag{51}$$

Once this is specified, the construction is completely analogous to the previous case. Expectation value functions are again defined as

$$e_A(\rho) = \operatorname{Tr}(\rho A); \qquad \rho \in \mathcal{D}, \tag{52}$$

while dynamics is defined through the Poisson tensor Ω and other physical properties as the uncertainty relations are encoded again in the tensor G.

5. – Interference in the Ehrenfest picture

5˙1. *Describing interference on $\mathcal{D}$.* – In the sections above we have been able to address some of the problems which arise when we formulate Quantum Mechanics in the Ehrenfest picture. In particular we have been able to define the dynamics and the uncertainty relations in terms of geometric objects which are defined either on the projective space $\mathcal{P}$ associated to the Hilbert space $\mathcal{H}$ or on the space of density operators $\mathcal{D}$.

Our final exercise addresses the problem of formulating interference phenomena within the framework. Consider then that we are given a pair of pure states ρ_1 and ρ_2 and that we want to find a method to combine them into a new pure state. Thus we must be able to define a procedure to combine two rank-one projectors into a new one. In order to do that, we need to fix a fiducial projector P_0 which will allow us to consider the relative phases which are essential to describe the interference process, diffraction or also the composition of light polarization.

Consider thus, given ρ_1, ρ_2 and P_0 as above, and $p_1, p_2 \in [0, 1]$ with $p_1 + p_2 = 1$, the operator

$$\rho = p_1\rho_1 + p_2\rho_2 + \frac{\sqrt{p_1 p_2}}{\operatorname{Tr}(\rho_1 P_0 \rho_2 P_0)}(\rho_1 P_0 \rho_2 + \text{h.c.}). \tag{53}$$

It is straightforward to prove that, with the conditions above, ρ is also a pure state, *i.e.*,

$$\rho^2 = \rho; \qquad \mathrm{Tr}\,\rho = 1.$$

Besides, it is simple to check that

$$\rho_1 \rho \rho_1 = p_1 \rho_1; \qquad \rho_2 \rho \rho_2 = p_2 \rho_2.$$

Notice that this composition law may be considered to provide us with a purification of the state $\rho = p_1\rho_1 + p_2\rho_2$ when the two pure states are orthogonal, and the projection on P_0 of both is different from zero, *i.e.*

$$\rho_1\rho_2 = 0; \qquad P_0\rho_1 \neq 0; \qquad P_0\rho_2 \neq 0.$$

When the two pure states ρ_1 and ρ_2 are not orthogonal

$$\rho = p_1\rho_1 + p_2\rho_2 + \frac{\sqrt{p_1p_2}}{\mathrm{Tr}(\rho_1 P_0 \rho_2 P_0)}(\rho_1 P_0 \rho_2 + \text{h.c.})W^{-1}, \tag{54}$$

where

$$W = 1 + \frac{\sqrt{p_1p_2}}{\mathrm{Tr}(\rho_1 P_0 \rho_2 P_0)}\,\mathrm{Re}(\rho_1 P_0 \rho_2 + \text{h.c.}). \tag{55}$$

To summarize the construction, we can say that having chosen a fiducial projector P_0, we are able to define a composition procedure of pure states which is an inner operation. For further details on this issue, we refer the interested reader to [30] and [27]. In the following we will study the geometrical meaning of the superposition procedure.

The projector P_0 we introduced plays the rôle of the Pancharatnam connection (see [31, 32]) which encodes the geometrical description of Berry phase (see [33-36]). Indeed, it provides a way to lift the physical states from the complex projective space into the Hilbert space. Once we have vectors in the Hilbert space, it is straightforward to evaluate the transition probability from one vector to another. In brief, we choose the fiducial projector as the rank one projector on a vector $|\psi_0\rangle \in \mathcal{H}$:

$$P_0 = \frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0|\psi_0\rangle}\,, \tag{56}$$

and then we are able to associate to the rank-one projector ρ_1 (respectively, ρ_2) the vector

$$|\psi_1\rangle = \frac{1}{\sqrt{\langle\psi_0|\psi_0\rangle}}\rho_1|\psi_0\rangle, \qquad |\psi_2\rangle = \frac{1}{\sqrt{\langle\psi_0|\psi_0\rangle}}\rho_2|\psi_0\rangle. \tag{57}$$

The transition probability between states ρ_1 and ρ_2 can be defined as

$$\mathcal{P}_{1-2} = |\langle\psi_1|\psi_2\rangle|^2 = \frac{\langle\psi_0|\rho_1\rho_2|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} = \mathrm{Tr}(\rho_1 P_0 \rho_2). \tag{58}$$

Then, with that result, the composition of the two states $|\psi_1\rangle$ and $|\psi_2\rangle$ allows us to describe properly the interference phenomena.

5˙2. *Example: the case of a two-level system.* – If we consider now the example of the two level system, we know that the projective space is diffeomorphic to the two-dimensional sphere S^2. If we want to define a linear structure on the sphere with the help of the projector P_0, we must exclude the points which are orthogonal to $|\psi_0\rangle$. We consider thus as set of representable states

$$V = S^2 - \{P_0^\perp\}.$$

The linear structure that we are defining on V is analogous to the one we obtain if we consider a point $s_0 \in S^2$, the corresponding tangent space $T_{s_0}S^2$; and with the help of any second-order differential equation on S^2 we define the time-one map to the sphere by means of the flow $\Phi : \mathbb{R} \times TS^2 \to TS^2$, *i.e.*:

$$\Phi(t, s_0, v)|_{t=1}; \qquad v \in T_{s_0}S^2.$$

Then, to any point in $s \in S^2$ (except the focal point of s_0, this is the reason to exclude $P_0^\perp$), we can associate a vector v in the tangent space $T_{s_0}S^2$:

$$s = \Phi(t = 1, s_0, v); \qquad S^2 \ni s \leftrightarrow v \in T_{s_0}S^2. \tag{59}$$

It is natural to consider a particular case for this second-order differential equation, as is the geodetic motion defined on the sphere. Thus the mapping Φ corresponds to the exponential mapping associated with the Riemannian structure of the projective space.

Then, given two arbitrary points $s_1, s_2 \in V$, we can associate a third element:

$$\begin{cases} s_1 = \Phi(t = 1, s_0, v_1) \\ s_2 = \Phi(t = 1, s_0, v_2) \end{cases} \Rightarrow s_1 \star s_2 = \Phi(t = 1, s_0, v_1 + v_2). \tag{60}$$

Once the linear structure has been implemented, the description of interference phenomena reduces to incoporate the scalar product of the physical states. Within our new framework, this can be accomplished by using the tensors $G_{\mathcal{P}}$ and $\Omega_{\mathcal{P}}$ defined in eqs. (25) and (26). We can define thus

$$(s_1, s_2) := G_{\mathcal{P}}(v_1, v_2) + i\Omega_{\mathcal{P}}(v_1, v_2). \tag{61}$$

Summarizing: on the projective space $\mathcal{P} \sim S^2$ minus the focal point to a fiducial point s_0, we can induce a vector space structure by using the linear structure of the vector space $T_{s_0}S^2$. Clearly, if two different fiducial points s_0, s_0' are used, we induce two alternative linear structures on the space S^2 excluding the two focal points. The transition function from one linear structure to the other defines a non-linear map. This construction shows the importance of alternative linear structures in Quantum Mechanics and how the usual linear structure of the Hilbert space formalism is an ingredient chosen by the observer, via the fiducial point used as reference for the interference phenomena.

* * *

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