

DIFFERENTIAL GEOMETRY OF DENSITY STATES

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We consider a geometrization, i.e., we identify geometrical structures, for the space of density states of a quantum system. We also provide few comments on a possible application of this geometrization for composite systems.

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1. Introduction

The notions of “states” and “observables” are fundamental in quantum mechanics. The space of states is usually assumed to be a vector space due to the introduction by Dirac [1] of the superposition principle as a fundamental principle of quantum theory. It is true however that one may consider superposition rules of solutions also for nonlinear evolution equations [2], this would give rise to a dynamical version of superposition (i.e., all superpositions of solutions for a given evolution equation represent new solutions).

The interpretation of wave functions as probability amplitudes suggested that the state space be identified as a Hilbert space, i.e., a vector space with an inner product.

The superposition principle, when applied to product states of composite systems, gives rise to the fundamental aspects of quantum nonseparability. In fact,

Schrödinger [3] had identified entanglement as a characteristic ingredient of quantum multipartite systems; superposition appears in classical wave phenomena and we have water waves and sound waves, but quantum entanglement is totally new.

While this entanglement has many observed consequences, it becomes spectacularly manifest in the violation of Bell's inequality. A particular use of it was the construction of "coherent state" of photons to represent electromagnetic fields.

Usually the implementation of the superposition principle at the level of solutions of evolution equations requires these equations to be linear. Some limitations arise from superselection rules but this will not concern us here.

In spite of this fundamental principle, usually one identifies states with rays generated by Hilbert space vectors rather than with the vectors themselves. This identification requires some additional ingredient to be able to discuss interference phenomena within the framework of rays. This becomes more evident if we use the identification of states as given by rank-one projectors, indeed, the usual superposition rule of two of these projectors will give, in general, as a result an operator of rank two. A way to handle this problem has been proposed recently [4], see also in this connection the recent paper [5]. A net result of the trading of vectors with equivalence classes is that we have a carrier space for quantum evolution which is not a linear space any more but a differential manifold (the complex projective space).

As for "observables", they are usually associated with measure operations. Measurements are described by means of Hermitian operators and often introduced as additional independent ingredients for the description of quantum phenomena. Even though Hermitian operators do not constitute an associative algebra, one usually considers them as part of the algebra of operators acting on the Hilbert space of quantum vectors. In the early times [6] of quantum mechanics, to have a binary product within the space of Hermitian operators, the Jordan product was introduced; it is a commutative product but not associative. By mapping Hermitian operators into the Lie algebra of the unitary group we get a binary product, the commutator or Lie product, which is a bilinear inner composition rule. These two products are enough to capture the essential ingredients of the measurement rules.

From what we have said about the identification of physical states with points of the complex projective space (associated with the Hilbert space \mathcal{H}), it is clear that the manifold structure of this space requires that we replace all objects, whose definition depends on the existing linear structure on \mathcal{H} , with "tensorial objects", i.e., geometrical entities which preserve their meaning under general transformations and not just linear ones. This "tensorial" viewpoint has been encoded into the differential-geometric approach to quantum mechanics which has been undertaken by a large number of physicists [7]. For a recent textbook treatment, we refer to the nice book by Chruściński and Jamiołkowski [8].

Bearing in mind these last remarks, in this paper we shall consider the Hilbert space \mathcal{H} as a real differential manifold with additional structures carrying an action of the unitary group. To let the geometrical structures to emerge neatly

without the technicalities due to the infinite dimension we shall restrict ourselves to finite-dimensional Hilbert spaces.

Therefore, the differential-geometric point of view is implemented by considering our relevant spaces as real differential manifolds. The complex structure of the standard Hilbert space is considered to be an additional structure on the real differential manifold.

This paper is addressed to theoretical physicists at home with the geometrical structures employed within the geometrical approach to classical mechanics.

2. The space of state vectors as a differential manifold

Starting with the complex Hilbert space \mathcal{H} , to deal with its real differential structure, we consider its “realification” $\tilde{\mathcal{H}}$ with the additional structures arising from the Hermitian inner product, i.e., the real part which defines a positive definite Riemannian structure (Euclidean product) g , the imaginary part defining a nondegenerate skew symmetric bilinear product which is a symplectic structure ω and a map connecting the two which corresponds to the multiplication by the imaginary unit, the complex structure J satisfying the properties $J^2 = -\mathbf{1}$ and $g(x, y) = \omega(Jx, y)$.

These three structures join together to define the Hermitian inner product

$$h(x, y) = g(x, y) + i\omega(x, y). \tag{1}$$

To turn these entities into tensors, we consider x, y as vector fields on the manifold $\tilde{\mathcal{H}}$ while Eq. (1) is thought of as the evaluation on vectors in $T_\psi\tilde{\mathcal{H}}$ at the point $\psi \in \tilde{\mathcal{H}}$. More specifically vector fields, $X : \tilde{\mathcal{H}} \rightarrow T\tilde{\mathcal{H}} \Leftrightarrow \tilde{\mathcal{H}} \times \tilde{\mathcal{H}}$, and 1-forms $\alpha : \tilde{\mathcal{H}} \rightarrow T^*\tilde{\mathcal{H}} \Leftrightarrow \tilde{\mathcal{H}} \times \tilde{\mathcal{H}}^* \Leftrightarrow \tilde{\mathcal{H}} \times \tilde{\mathcal{H}}$ will be identified with their second component. $\tilde{\mathcal{H}}$ and $\tilde{\mathcal{H}}^*$ are identified by means of the Euclidean inner product, associated with g .

By using collective coordinates $\{x^j\}$, we would have

$$\begin{aligned} g &= g_{jk}dx^j \otimes dx^k, \\ \omega &= \omega_{jk}dx^j \wedge dx^k, \\ J &= g^{jk}\omega_{kl}dx^l \otimes \frac{\partial}{\partial x^j}, \quad j, k = \{1, 2, \dots, 2n\}, \end{aligned} \tag{2}$$

with the property $J^2 = -\mathbf{1}$.

It is not difficult to show that if formula (1) defines a Hermitian product we have

$$(a) \quad g(Jx, Jy) = g(x, y), \quad \forall x, y, \quad g(Jx, y) + g(x, Jy) = 0, \tag{3}$$

$$(b) \quad \omega(Jx, Jy) = \omega(x, y), \quad \omega(Jx, y) + \omega(x, Jy) = 0, \tag{4}$$

i.e., J generates both finite and infinitesimal transformations which are orthogonal and symplectic.

The vector space structure of \mathcal{H} is associated with the dilation vector field Δ given by

$$\Delta = x^j \frac{\partial}{\partial x^j} \quad (5)$$

which is also known as Liouville vector field or the Euler operator.

By using the $(1-1)$ -tensor field J we may define another vector field $\Gamma = J(\Delta)$. These two vector fields commute and generate a foliation of $\tilde{\mathcal{H}} - \{0\}$ in terms of two-dimensional real vector spaces (strictly speaking, leaves are diffeomorphic with $\mathbb{R}^2 - \{0\}$).

By means of Δ one defines homogeneous polynomial functions of degree k by requiring $\Delta \cdot f = kf$. This definition has the advantage of being coordinate independent, i.e., we may even perform nonlinear transformations of coordinates.

The symplectic structure ω defines a Poisson tensor

$$\Lambda = \Lambda^{jk} \frac{\partial}{\partial x^j} \wedge \frac{\partial}{\partial x^k} \quad (6)$$

with

$$\Lambda^{jk} \omega_{kl} = \delta_l^j, \quad \Lambda^{jk} = -\Lambda^{kj}. \quad (7)$$

It is also possible to consider the inverse of g , namely,

$$G = G^{jk} \frac{\partial}{\partial x^j} \otimes \frac{\partial}{\partial x^k} \quad (8)$$

with

$$G^{jk} = G^{kj} \quad \text{and} \quad G^{jk} g_{kl} = \delta_l^j. \quad (9)$$

They are related by $G = J \cdot \Lambda$. These tensors Λ and G allow us to define a Poisson bracket and a Riemann–Jordan bracket [9] on smooth functions in $\mathcal{F}(\tilde{\mathcal{H}})$ by setting, respectively,

$$\{f, g\} = \Lambda(df, dg) = \Lambda^{kj} \left(\frac{\partial f}{\partial x^j} \frac{\partial g}{\partial x^k} \right) \quad (10)$$

and

$$(f, g) = G(df, dg) = G^{kj} \left(\frac{\partial f}{\partial x^j} \frac{\partial g}{\partial x^k} \right). \quad (11)$$

By using Λ , we may consider the group of transformations which preserve both Λ and Δ , we get in this way the group of real linear symplectic transformations. By replacing Λ with G , we define the group of real linear orthogonal transformations. The intersection of these two invariance groups defines the group of unitary transformations, denoted by $U(n)$ when $\tilde{\mathcal{H}}$ is assumed to be of (real) dimensions $2n$.

Symmetric tensor fields $t = t_{kj} dx^j \otimes dx^k$ are converted into quadratic functions f_t by considering

$$2f_t = t(\Delta, \Delta) = t_{jk} x^j x^k, \quad (12)$$

and similarly for higher-order tensors. For skew-symmetric 2-tensors, we may define for $\gamma = \gamma_{jk} dx^j \wedge dx^k$, $2f_\gamma = \gamma(\Delta, J(\Delta))$. (The factor 2 is very convenient if

at some point we want to identify our function with the energy, when it is the case.) When the skew-symmetric 2-tensor coincides with the symplectic structure, the corresponding function is the Hamiltonian function generating the one-parameter group of unitary transformations which consists of multiplication by a phase.

Any linear operator $A : \tilde{\mathcal{H}} \rightarrow \tilde{\mathcal{H}}$ can be converted into a $(1 - 1)$ -tensor field by setting

$$T_A = A_k^j dx^k \otimes \frac{\partial}{\partial x^j} \tag{13}$$

or into a vector field

$$X_A = T_A(\Delta) = A_k^j x^k \frac{\partial}{\partial x^j}, \tag{14}$$

along with $Y_A = T_A(J(\Delta))$. If A hermitian operator, X_A corresponds to the gradient vector field, while Y_A corresponds to the Hamiltonian vector field associated with the expectation value of the operator.

The association of A with T_A is an associative algebra isomorphism, while the association of A with X_A allows one to capture only the Lie algebra structure.

By using g and ω , it is possible to associate a complex-valued quadratic function on $\tilde{\mathcal{H}}$ with any linear transformation A by setting

$$2f_A = g(\Delta, T_A(\Delta)) + i\omega(\Delta, T_A(\Delta)) = g_{jk} A_l^k x^j x^l + i\omega_{jk} A_l^k x^j x^l, \tag{15}$$

equivalently, on \mathcal{H} , we could write $2f_A(\psi) = \langle \psi | A\psi \rangle$.

All our constructions have been written in an implicit form to exhibit their independence of the chosen coordinates and to hint at the fact that they remain true at the level of infinite-dimensional Hilbert spaces, whenever the relative tensors are defined.

Because we shall be mainly interested in the “realification” of operations taking place on the complex Hilbert space, we shall always consider $(1 - 1)$ -tensor fields T_A associated with complex-linear operators, i.e., $T_A \cdot J = J \cdot T_A$

This amounts to consider only complex linear transformations, i.e. only real representations of $GL(n, \mathbb{C})$.

It is now a simple result following from computations that for complex-valued functions

$$\{f_A, f_B\} = -if_{[A,B]} \tag{16}$$

and

$$(f_A, f_B) = 2f_{(AB+BA)}, \tag{17}$$

i.e., for quadratic functions associated with complex linear operators, we recover the Lie product and the Jordan product by using the Poisson tensor Λ and the Riemannian tensor G , respectively.

We have now the possibility of characterizing canonical transformations in a way that turns out to be useful when dealing with quantum gates. We recall that canonical transformations are implicitly defined by the property of leaving the

Poisson brackets invariant. However, when dealing with a transformation from (q, p) to (Q, P) variables, a different characterization is obtained by requiring that

$$p^a dq_a - P^b dQ_b = dS(q, Q).$$

In the extended formalism [10] this would be

$$(p^a dq_a - H dt) - (P^b dQ_b - K dt) = dW(q, Q; t).$$

If we want to make contact with standard Hilbert space approach, we may use complex coordinates, say $\psi = q + ip$, $\phi = Q + iP$, and we may write previous equations in the form

$$\frac{1}{2} i [\phi^k d\phi_k^* + \phi_k^* d\phi^k - 2d\phi^k \phi_k^* - (\psi^k d\psi_k^* + d\psi^k \psi_k^*) + 2d\psi^k \psi_k^*] = dS(\psi^k, \phi^k),$$

or directly

$$i(d\psi^k \psi_k^* - d\phi^k \phi_k^*) = dS(\phi^k, \psi^k).$$

This equation may be spelled out into

$$i\psi_k^* = \frac{\partial S}{\partial \psi^k}, \quad -i\phi_k^* = \frac{\partial S}{\partial \phi^k}.$$

REMARK. By making different choices of the independent variables, say instead of ψ, ϕ we could use (ψ, ϕ^*) , (ψ^*, ϕ^*) , (ψ^*, ϕ) , we would have different expressions for the generating functions [10]. If we require the transformation to be linear, we start with a quadratic generating functions S . In general, as functions of complex variables, they should be at least analytic in the relevant variables. By requiring that the resulting transformation preserves J we find that eventually our transformations will be unitary. If $\phi^k = U_j^k \psi_j$ is a unitary transformation connecting two different bases, one obtains as a generating function $S = i\phi_k^* U_j^k \psi_j$. However, one should bear in mind that the class of canonical transformations is much larger than the class of unitary transformations, and moreover they will be well defined also on the space of rays, the complex projective space.

In the simplest case of $\mathcal{H} = \mathcal{C}^2$, we may write few generating functions which describe some well-known quantum gates.

For beam splitter or Hadamard gate, we have

$$S_H = \frac{i}{\sqrt{2}} (\phi_1^* \psi^1 + \phi_2^* \psi^1 + \phi_1^* \psi^2 - \phi_2^* \psi^2),$$

similarly for the phase gate $S = i\phi_1^* \psi^1 - \phi_2^* \psi^2$, and for the phase-shift we have $i(\phi_1^* \psi^1 + e^{i\theta} \phi_2^* \psi^2)$.

As it is well known, generating functions add to represent the composition of transformations. Having represented gates in terms of generating functions, we are no more restricted to linear spaces.

From now onwards, whenever there is no danger of confusion we shall also make use, in the algebraic or linear setting, of complex coordinates so that the

comparison with standard quantum mechanics becomes more transparent. While, whenever we deal with nonlinear transformations or tensorial aspects of quantum mechanics or differential geometrical aspects, our treatment only considers real differential structures.

3. The unitary group as a group of canonical transformations: momentum map

The group of linear transformations preserving the triple (g, ω, J) is the unitary group denoted by $U(n)$, the associated Lie algebra will be denoted $u(n)$. If we denote by $\mathcal{X}(\tilde{\mathcal{H}})$ the Lie algebra of vector fields on $\tilde{\mathcal{H}}$, we have a Lie algebra homomorphism $u(n) \rightarrow \mathcal{X}(\tilde{\mathcal{H}})$. With any Hermitian operator A we may associate a vector field

$$X_A = -\frac{i}{\hbar} T_A(\Delta), \tag{18}$$

which is the infinitesimal generator of the one-parameter group of unitary transformations

$$U(\alpha) = e^{-i\alpha A/\hbar}, \tag{19}$$

where the parameter α is such that the product of the physical dimensions of α and A has the dimension of an action. With a slight abuse of notation, denoting by $iu(n)$ the set of Hermitian operators, we have a map linear in the second argument

$$F : \tilde{\mathcal{H}} \times iu(n) \rightarrow \mathbb{R} \tag{20}$$

specifically

$$2F(\psi, A) = \langle \psi | A\psi \rangle. \tag{21}$$

It has the property

$$\{F(A), F(B)\} = iF([A, B]), \tag{22}$$

where $F(A) : \tilde{\mathcal{H}} \rightarrow \mathbb{R}$ is defined out of F in an obvious way. By using the Cartesian property of maps, $\mathcal{F}(\tilde{\mathcal{H}} \times U(n)) = \mathcal{F}(\tilde{\mathcal{H}}, \text{Lin}(U(n), \mathbb{R}))$, we may define also

$$\hat{F} : \tilde{\mathcal{H}} \rightarrow u^*(n) = \text{Lin}(u(n), \mathbb{R}). \tag{23}$$

This map is usually called the momentum map associated with the symplectic action of the group $U(n)$ on $\tilde{\mathcal{H}}$.

It is useful to present explicitly the momentum map associated with $U(n)$ acting on $\tilde{\mathcal{H}}$, i.e., the complex Hilbert space, in terms of Dirac notation and using the identification of $u(n)$ with its dual by means of the Cartan–Killing metric structure on $u(n)$ we have

$$\hat{F}(\psi) = -i | \psi \rangle \langle \psi |. \tag{24}$$

We find the remarkable result that the unit sphere of the Hilbert space can be imbedded into $u^*(n)$ equivariantly with respect to the coadjoint action.

As a matter of fact, it is now possible to foliate $\tilde{\mathcal{H}} - \{0\}$ with the involutive distributions of the vector fields Δ and $J(\Delta)$, to obtain as quotient a real differential

manifold, diffeomorphic with the complex projective Hilbert space $\mathcal{P}(\tilde{\mathcal{H}})$. It is not difficult to show that $J(\Delta)$ is the Hamiltonian vector field associated with the function $f_1 = \frac{1}{2}\langle\psi | \psi\rangle$.

If we replace the evaluation function $2f_A(\psi) = \langle\psi | A\psi\rangle$ with the expectation value of A at ψ , say

$$\tilde{f}_A(\psi) = \frac{\langle\psi | A\psi\rangle}{\langle\psi | \psi\rangle}, \quad (25)$$

we find that $\tilde{f}_A(\psi)$ is invariant under Δ and $J(\Delta)$. The invariance under Δ is obvious. For the invariance under $J(\Delta)$, we use the fact that $J(\Delta)$ is the Hamiltonian vector field associated with f_1 and $\{f_1, f_A\} = 0$ from (22). Thus the algebra of functions defined by the expectation values of Hermitian operators projects onto the quotient space of $\tilde{\mathcal{H}} - \{0\}$ with respect to the foliation defined by Δ and $J(\Delta)$. This algebra separates the points of the quotient and therefore completely determines it.

REMARK. Equivalently to obtain a differential manifold diffeomorphic with the quotient complex projective space we consider the Poisson bracket on $\tilde{\mathcal{H}}$ and notice that the centralizer of $2f_1 = \langle\psi | \psi\rangle$ in $\mathcal{F}(\tilde{\mathcal{H}}, \mathcal{R})$ is a Poisson subalgebra. The Poisson bracket can be extended to complex-valued function and contains the set of quadratic complex-valued functions associated with complex linear operators $A : \mathcal{H} \rightarrow \mathcal{H}$, i.e., $\tilde{f}_A(\psi) = \frac{\langle\psi | A\psi\rangle}{\langle\psi | \psi\rangle}$, more generally $\tilde{f}(\psi) = \frac{f(\psi)}{\langle\psi | \psi\rangle}$. This Poisson algebra coincides with the Poisson algebra of complex-valued functions defined on the complex projective space. Indeed, each function $\tilde{f}_A(\psi)$ is invariant under the infinitesimal action of Δ and $J(\Delta)$. The Poisson bracket on the complex projective space defines a symplectic structure. The complex structure J on $\tilde{\mathcal{H}}$ induces a complex structure on $\mathcal{P}\tilde{\mathcal{H}}$ by setting $\hat{F}_*(\tilde{J}df) := J(\hat{F}_*(df))$ for any function on $\mathcal{P}\tilde{\mathcal{H}}$. The invariance of J under the action of Δ and $J(\Delta)$ shows that $J(\hat{F}_*(df))$ is the pull-back of a 1-form on $\mathcal{P}\tilde{\mathcal{H}}$ and therefore the left-hand side (i.e., \tilde{J}) is well defined. Out of the symplectic structure and \tilde{J} on $\mathcal{P}\tilde{\mathcal{H}}$ we can construct a Kähler structure.

The projection $\tilde{F} : \tilde{\mathcal{H}} - \{0\} \rightarrow \mathcal{P}\tilde{\mathcal{H}}$, written in explicit form by means of the momentum map associated with unitary transformations, and the required invariance under Δ and $J(\Delta)$, has the form

$$\tilde{f}(\psi) = -i \frac{|\psi\rangle\langle\psi|}{\langle\psi | \psi\rangle}.$$

A connection 1-form for this projection can be given by requiring that Δ and $J(\Delta)$ are fundamental vector fields.

The connection 1-form can be written in compact form by using Dirac notation

$$\theta = \frac{\langle\psi | d\psi\rangle}{\langle\psi | \psi\rangle}.$$

It is now sufficient to show that

$$\theta(J(\Delta)) = i, \quad \theta(\Delta) = 1.$$

By using real coordinates, say, $\psi = (q + ip)$, we find

$$\frac{\psi^* d\psi}{\langle \psi | \psi \rangle} = \frac{(q - ip)d(q + ip)}{q^2 + p^2} = \frac{q dq + p dp}{q^2 + p^2} + i \frac{q dp - p dq}{q^2 + p^2},$$

while

$$\Delta = q \frac{\partial}{\partial q} + p \frac{\partial}{\partial p}, \quad J(\Delta) = q \frac{\partial}{\partial p} - p \frac{\partial}{\partial q}.$$

Horizontal vectors are those vectors in $T_\psi \mathcal{H}$ which are in the kernel of θ . Usually one avoids dealing with additional terms due to Δ by restricting very soon all considerations to the unit sphere $S(\mathcal{H}) = \{\psi \in \mathcal{H} \mid \langle \psi | \psi \rangle = 1\}$.

Our choice is dictated by the desire to keep separate notions which depend on the chosen Hermitian structure from those which do not rely on it.

It is now possible to write a Hermitian tensor which is a metric on horizontal vectors or equivalently on $\mathcal{P}\mathcal{H}$ (where it becomes the well-known Fubini–Study metric tensor [13]) by setting

$$\frac{(\psi \wedge d\psi)^2}{\langle \psi | \psi \rangle^2} = \left\{ \frac{\langle d\psi | d\psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \psi | d\psi \rangle \langle d\psi | \psi \rangle}{\langle \psi | \psi \rangle^2} \right\}.$$

(The use of vector-valued differential forms may be very convenient for quick algebraic manipulations, some aspects are dealt with in [12]).

The real part of this Hermitian tensor will be the Riemannian metric while the imaginary part will be the symplectic structure on $\tilde{\mathcal{P}}\mathcal{H}$.

The trick of restricting everything to the unit sphere $S(\mathcal{H}) \subset \mathcal{H}$ hides the fact that the pull-back of the Fubini–Study metric on $\tilde{\mathcal{P}}\mathcal{H}$ is only conformally related to the Euclidean metric on $\tilde{\mathcal{H}}$.

4. Density states

Our imbedding of the complex projective space into $u^*(n)$ is achieved by setting, for any equivalence class $[\psi]$,

$$[\psi] \rightarrow -i \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}, \tag{26}$$

which clearly does not depend on the representative chosen within $[\psi]$.

By introducing the rank-one projector ρ_ψ ,

$$\rho_\psi = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}, \tag{27}$$

we can write in standard notation

$$f_A(\psi) = \text{tr } \rho_\psi A = \text{Tr } [[\psi] (iA)]. \tag{28}$$

Let us summarize the situation.

Out of the action of the unitary group on $\tilde{\mathcal{H}}$, we have constructed an imbedding of the complex projective space into the dual of the Lie algebra of the unitary

group, i.e., by means of the momentum map. The target space of this map is a linear space, therefore, we have imbedded our nonlinear differential manifold into a linear space, allowing us to consider linear combinations of points in the image and therefore to go beyond rays, or pure states. The equivariance of the momentum map means that any unitary evolution on the Hilbert space (associated with the Schrödinger equation) will give rise to a unitary evolution on $u^*(n)$ (associated with the von Neumann equation) [11].

The interpretation of $f_A([\psi])$ as an expectation value allows us to consider probability distributions or averaging A on a set of states with appropriate weights. We may thus consider the average

$$\sum_k p_k \text{Tr } \rho_k A = \text{Tr } \rho A \quad (29)$$

with

$$p_k \geq 0 \quad \forall k, \quad \sum_k p_k = 1, \quad \rho_k = \rho_k^\dagger, \quad \rho_k^2 = \rho_k, \quad \text{tr } \rho_k = 1.$$

Out of points $(\rho_1, \rho_2, \dots, \rho_k, \dots)$ in the image of the complex projective space, we have formed $\sum_k p_k \rho_k$ which can be identified with an element in $u^*(n)$. The probabilistic interpretation requires that we deal only with convex combinations.

Clearly we can extend our original Poisson bracket on expectation values from $f_A(\psi)$ to $f_A(\rho) = \sum_k p_k f_A(\psi_k)$ simply by linearity

$$\{f_A, f_B\}(\rho) := \sum_k p_k f_{i[A, B]}(\psi_k) = \sum_k p_k \{f_A, f_B\}(\psi_k). \quad (30)$$

Similarly, the Riemann–Jordan bracket can be extended by linearity

$$(f_A, f_B)(\rho) := \sum_k \rho_k (f_A, f_B)(\psi_k). \quad (31)$$

From now onwards we shall denote all convex combinations of pure states as $\mathcal{D}(\mathcal{H})$ and call them density states.

5. Geometrical structures on the space of density states

We shall now consider the mathematical structures available on $\mathcal{D}(\mathcal{H})$. When we want to use differential-geometric properties of $\mathcal{D}(\mathcal{H})$, we shall always consider it as a real differential manifold with boundary and denote it as $\tilde{\mathcal{D}}(\tilde{\mathcal{H}})$ imbedded into the real vector space $u^*(n)$.

On $\tilde{\mathcal{D}}(\tilde{\mathcal{H}})$ there is a Poisson tensor $\tilde{\Lambda}$ associated with brackets (30) and a metric tensor \tilde{G} associated with bracket (31). Obviously $\tilde{\Lambda}$ is degenerate, the kernel being associate with Casimir functions. If we use expectation values $f_A(\rho)$, we can define a partial complex structure by setting [14]

$$J\tilde{G}(df_A) := \tilde{\Lambda}(df_A), \quad (32)$$

showing that gradient-vector fields associated with Casimir functions must be in the kernel of J . Therefore $J^2 = -\mathbf{1}$ only when we restrict it to combinations of

Hamiltonian vector fields. We also notice that Hamiltonian vector fields are always tangent to the topological boundary of $\mathcal{D}(\tilde{\mathcal{H}})$.

In summary, we may say that the tangent space of $\mathcal{D}(\tilde{\mathcal{H}})$, in its internal points, is spanned by the Hamiltonian vector fields and the gradient vector fields associated with Casimir functions.

As $\mathcal{D}(\tilde{\mathcal{H}})$ is the union of symplectic orbits of the coadjoint action of $U(n)$ on $u^*(n)$, on each orbit there is a symplectic structure defined by projecting from the group onto the orbit [15],

$$\omega_\rho = d \operatorname{Tr}(\rho U^\dagger dU) = -\operatorname{Tr}(\rho U^\dagger dU \wedge U^\dagger dU). \tag{33}$$

The boundary is a stratified manifold, being the union of symplectic orbits of different dimensions passing through density matrices of not maximal rank. It should be remarked that while the two-form is well defined on the orbit, the one-form $U^\dagger dU$ is a Lie algebra valued one-form on the unitary group $U(n)$ which does not descent to the orbit. It is not difficult to show that the kernel of ω_ρ , $\operatorname{Ker} \omega_\rho$, is spanned by infinitesimal generators of the isotropy group (or stability group) of ρ under the coadjoint action of the unitary group.

Previous considerations show that $\mathcal{D}(\tilde{\mathcal{H}})$ has an inverse image under the momentum map $\mu : T^*U(n) \rightarrow u^*(n)$. We may consider $\mu^{-1}(\mathcal{D}(\tilde{\mathcal{H}}))$ and use the geometric structures available on $T^*U(n)$ which is diffeomorphic with a subgroup of $GL(n, \mathcal{C})$. In particular, $T^*SU(n)$ is symplectomorphic with the group $SL(n, \mathcal{C})$ considered as a Drinfeld double [16].

In particular, any torus action coming from a Cartan subalgebra in $U(n)$ gives rise to a complex torus action on $T^*U(n)$, no more unitary. This violation of unitarity seems to have an interpretation in terms of quantum measurements and provides a possible useful description of the wave function collapse [17]. We shall develop these considerations elsewhere.

6. Example: a two-level system

In this section, we shall describe our previous constructions in terms of $\mathcal{H} = \mathbb{C}^2 \equiv \mathbb{R}^4$, i.e., a two-level quantum system.

We introduce an orthogonal basis $|e_1\rangle$ and $|e_2\rangle$ and any vector $|\psi\rangle$ will be decomposed into $|\psi\rangle = z_1 |e_1\rangle + z_2 |e_2\rangle$, therefore \mathbb{C}^2 will be parametrized by complex coordinates (z_1, z_2) . To deal with its realification \mathbb{R}^4 , we consider also real coordinates defined by the formulae $z_1 = q_1 + ip_1$, $z_2 = q_2 + ip_2$.

The unitary group $U(2)$ is realized by requiring that it preserves the quadratic function $z_1^* z_1 + z_2^* z_2$, or equivalently, the quadratic function $q_1^2 + q_2^2 + p_1^2 + p_2^2$. The momentum map associated with the symplectic action of $U(2)$ on \mathcal{R}^4 is given by

$$\hat{F} : \mathcal{H} \rightarrow u^*(n),$$

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \rightarrow -i \begin{pmatrix} z_1 z_1^* & z_1 z_2^* \\ z_2 z_1^* & z_2 z_2^* \end{pmatrix}.$$

The multiplication by the imaginary unit i turns it into the infinitesimal generator of one-parameter group of unitary transformations.

Fundamental tensors for those examples are given by

- 1) $\Delta = p_1 \frac{\partial}{\partial p_1} + p_2 \frac{\partial}{\partial p_2} + q_1 \frac{\partial}{\partial q_1} + q_2 \frac{\partial}{\partial q_2},$
- 2) $J = dp_1 \otimes \frac{\partial}{\partial q_1} - dq_1 \otimes \frac{\partial}{\partial p_1} + dp_2 \otimes \frac{\partial}{\partial q_2} - dq_2 \otimes \frac{\partial}{\partial p_2},$
- 3) $J(\Delta) = p_1 \frac{\partial}{\partial q_1} - q_1 \frac{\partial}{\partial p_1} + p_2 \frac{\partial}{\partial q_2} - q_2 \frac{\partial}{\partial p_2}.$

Therefore, to have \hat{F} equivariant with respect to the infinitesimal action of Δ and $J(\Delta)$, we have to redefine the normalized momentum map

$$\tilde{F} : \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \rightarrow -i\rho_z = \frac{-i}{z_1 z_1^* + z_2 z_2^*} \begin{pmatrix} z_1 z_1^* z_1 z_2^* \\ z_2 z_1^* z_2 z_2^* \end{pmatrix}$$

with $i\rho_z \in u(n)$.

In terms of Pauli matrices, we find

$$i\rho_z = \frac{i}{2} (\sigma_0 + \vec{x}\vec{\sigma})$$

with identification

$$x_1 = \frac{z_1 z_2^* + z_1^* z_2}{z_1 z_1^* + z_2 z_2^*}, \quad x_2 = i \frac{z_1 z_2^* - z_1^* z_2}{z_1 z_1^* + z_2 z_2^*}, \quad x_3 = \frac{z_1 z_1^* - z_2 z_2^*}{z_1 z_1^* + z_2 z_2^*}$$

and, obviously, $x_1^2 + x_2^2 + x_3^2 = 1$.

It is quite clear that the pull-back of these functions to $\mathbb{R}^4 - \{0\}$ are invariant under the infinitesimal action of Δ and under the infinitesimal action of $J(\Delta)$.

The Hermitian tensor introduced in Section 3 has the form

$$(ds)^2 = \frac{dz_1^* dz_1 + dz_2^* dz_2}{z_1 z_1^* + z_2 z_2^*} - \frac{(z_1^* dz_1 + z_2^* dz_2)(z_1 dz_1^* + z_2 dz_2^*)}{(z_1 z_1^* + z_2 z_2^*)^2}$$

providing us with the Riemannian (real part) and symplectic two-form (imaginary part), on the complex projective metric space.

It is quite instructive to use real coordinates to write real and imaginary part of the previous Hermitian tensor.

We set, $a \in (1, 2)$,

$$z_a = q_a + ip_a, \quad H_a = \frac{1}{2} (p_a^2 + q_a^2), \quad d\varphi_a = \frac{q_a dp_a - p_a dq_a}{2H_a},$$

moreover $H = H_1 + H_2$.

We find

$$g_{\text{FS}} = \sum_a \left(\frac{dq_a \otimes dq_a + dp_a \otimes dp_a}{2H} - \frac{dH \otimes dH}{(2H)^2} - \frac{4(H_a d\varphi_a) \otimes (H_a d\varphi_a)}{(2H)^2} \right),$$

$$\omega_{\text{FS}} = \sum_a \frac{dq_a \wedge dp_a}{2H} - \frac{dH \wedge (2H_1 d\varphi_1 + 2H_2 d\varphi_2)}{(2H)^2}$$

$$= \sum_a \frac{1}{2} d \left(\frac{H_a d\varphi_a}{H} \right) = \frac{1}{2} \sum_a \left(\frac{dH_a \wedge d\varphi_a}{H} \right) - \frac{dH \wedge (H_1 d\varphi_1 + H_2 d\varphi_2)}{(H)^2}.$$

By computation we find that vertical vector fields are in the kernel of the symmetric tensor and of the skew-symmetric one:

$$g_{\text{FS}}(\Delta, \Delta) = 0, \quad g_{\text{FS}}(J(\Delta), J(\Delta)) = 0,$$

$$\omega_{\text{FS}}(\Delta) = 0, \quad \omega_{\text{FS}}(J(\Delta)) = 0.$$

In this example, we see very clearly that g_{FS} is only conformally related to the Euclidean product evaluated on horizontal vectors.

The projection (momentum map) relates the Poisson bracket on $S^2 \subset \mathbb{R}^3$ with the Poisson brackets on \mathbb{R}^4 it is a symplectic realization of Poisson brackets on \mathbb{R}^3 . By considering convex combinations, we get the unit ball out of the sphere S^2 , we have $\rho = \sum_k p_k \rho_k$. The space $\mathcal{D}(\mathbb{C}^2)$ would be represented by density states $\frac{1}{2}(\sigma_0 + \vec{x}\vec{\sigma})$ with $||\vec{x}|| \leq 1$. The topological boundary $\partial\mathcal{D}(\mathbb{C}^2) = \mathbb{C}P^1$, however, in higher dimensions it is not true that pure states coincide with the topological boundary of density states.

The Poisson bracket extended to $\mathcal{D}(\mathbb{C}^2) \subset \mathbb{R}^3$, i.e., to functions $f_A(\rho) = \text{Tr} \rho A$ for all Hermitian operators A , gives rise to the natural Poisson bracket on the dual of the Lie algebra. In the present case, it is the one associated with $SU(2)$, namely

$$\tilde{\Lambda} = x_1 \frac{\partial}{\partial x_2} \wedge \frac{\partial}{\partial x_3} + x_2 \frac{\partial}{\partial x_3} \wedge \frac{\partial}{\partial x_1} + x_3 \frac{\partial}{\partial x_1} \wedge \frac{\partial}{\partial x_2},$$

while the metric tensor on $su^*(2)$ is

$$\tilde{G} = \frac{\partial}{\partial x_1} \otimes \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \otimes \frac{\partial}{\partial x_2} + \frac{\partial}{\partial x_3} \otimes \frac{\partial}{\partial x_3}.$$

The resulting partial complex structure has the form

$$J = \frac{\partial}{\partial x_1} \otimes \frac{x_2 dx_3 - x_3 dx_2}{\sqrt{x_2^2 + x_3^2}} + \frac{\partial}{\partial x_2} \otimes \frac{x_3 dx_1 - x_1 dx_3}{\sqrt{x_1^2 + x_3^2}} + \frac{\partial}{\partial x_3} \otimes \frac{x_1 dx_2 - x_2 dx_1}{\sqrt{x_1^2 + x_2^2}}$$

$$= \left(x_3 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_3} \right) \otimes \frac{dx_1}{\sqrt{x_2^2 + x_3^2}} + \left(x_2 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_2} \right) \otimes \frac{dx_3}{\sqrt{x_1^2 + x_2^2}}$$

$$+ \left(x_1 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_1} \right) \otimes \frac{dx_2}{\sqrt{x_1^2 + x_3^2}}$$

and moreover

$$J(x_1 dx_1 + x_2 dx_2 + x_3 dx_3) = 0, \quad J\left(x_1 \frac{\partial}{\partial x_1} + x_2 \frac{\partial}{\partial x_2} + x_3 \frac{\partial}{\partial x_3}\right) = 0.$$

We notice that a two-form which provides a left inverse for Λ is given by

$$\omega = \frac{1}{x_1^2 + x_2^2 + x_3^2} (x_1 dx_2 \wedge dx_3 + x_2 dx_3 \wedge dx_1 + x_3 dx_1 \wedge dx_2)$$

showing that ω is not closed! Indeed, it should be closed only on each symplectic orbit.

The “quadratic” function associated with $A = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}$ is given by

$$\begin{aligned} f_A(\rho) &= \frac{1}{2} \text{Tr}(\sigma_0 + \vec{x}\vec{\sigma}) A \\ &= \frac{1}{2} x_3(a_1 - a_4) + \frac{1}{2} x_1(a_3 + a_2) + \frac{i}{2} x_2(a_2 - a_3) \end{aligned}$$

with corresponding Hamiltonian vector field

$$\begin{aligned} \tilde{\Lambda}(df_A) &= \frac{a_1 - a_4}{2} \left(x_2 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3} \right) + \frac{a_3 + a_2}{2} \left(x_3 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_3} \right) \\ &\quad + \frac{i(a_2 - a_3)}{2} \left(x_1 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_1} \right). \end{aligned}$$

By considering also the gradient vector field associated with Casimir function $\zeta = x_1^2 + x_2^2 + x_3^2$, we get

$$\tilde{\Delta} = \tilde{G}(d\zeta), \quad \tilde{\Delta} = x_1 \frac{\partial}{\partial x_1} + x_2 \frac{\partial}{\partial x_2} + x_3 \frac{\partial}{\partial x_3},$$

which along with the three rotation vector fields provides a basis for the module of vector fields on the unit ball.

A decomposition of a generic linear vector field on the unit ball can be achieved by using the basis $\{x_j \frac{\partial}{\partial x_k}\}$, $j, k \in \{1, 2, 3\}$.

7. Composite systems

The state space of a composite system is the tensor product of the state spaces of the component systems. If \mathcal{H}_A and \mathcal{H}_B are the Hilbert spaces of the component systems, the Hilbert space for the composite system is $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$.

Clearly, once \mathcal{H} has been built, we could use all constructions we have already performed in the previous sections. Here we would like to keep track of the component systems and of the geometrical structures pertaining to them. Instead of

general aspects, we shall concentrate directly on an example. We consider component systems to be two-level quantum systems, i.e., $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2 \equiv \mathbb{C}^4$.

If $\begin{vmatrix} z_1 \\ z_2 \end{vmatrix}$, $\begin{vmatrix} w_1 \\ w_2 \end{vmatrix}$ are state vectors for \mathcal{H}_A and \mathcal{H}_B , respectively, we have

$$\begin{vmatrix} z_1 \\ z_2 \end{vmatrix} \otimes \begin{vmatrix} w_1 \\ w_2 \end{vmatrix} = \begin{vmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{vmatrix} = \begin{vmatrix} z_1 w_1 \\ z_1 w_2 \\ z_2 w_1 \\ z_2 w_2 \end{vmatrix}.$$

The momentum map, which imbeds the complex projective space of the composite system into the Lie algebra of $U(4)$ is given by

$$\rho_u = \begin{vmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{vmatrix} \begin{vmatrix} u_1^* & u_2^* & u_3^* & u_4^* \end{vmatrix} = \begin{vmatrix} u_1 u_1^* & u_1 u_2^* & u_1 u_3^* & u_1 u_4^* \\ u_2 u_1^* & u_2 u_2^* & u_2 u_3^* & u_2 u_4^* \\ u_3 u_1^* & u_3 u_2^* & u_3 u_3^* & u_3 u_4^* \\ u_4 u_1^* & u_4 u_2^* & u_4 u_3^* & u_4 u_4^* \end{vmatrix}.$$

Using the representation of the density states for the component systems in terms of Pauli matrices, we find pure separable states for the composite system described by

$$\rho = \frac{1}{4}(\mathbf{1} + n_j \sigma_A^j \otimes \mathbf{1}_B + m_k \mathbf{1}_A \otimes \sigma_B^k + n_j m_k \sigma_A^j \otimes \sigma_B^k)$$

with $\|\vec{n}\|^2 = \|\vec{m}\|^2 = 1$.

In general, a density state will have the form

$$\rho = \frac{1}{4}(\mathbf{1} + p_j \sigma_A^j \otimes \mathbf{1}_B + q_k \mathbf{1}_A \otimes \sigma_B^k + r_{jk} \sigma_A^j \otimes \sigma_B^k)$$

with the condition $\sum_j (p_j^2 + q_j^2) + \sum_{j,k} r_{jk}^2 \leq 1$.

Matrices $i(\sigma_A^j \otimes \mathbf{1}_B)$, $i(\mathbf{1}_A \otimes \sigma_B^k)$, $i(\sigma_A^j \otimes \sigma_B^k)$ are a basis for the Lie algebra of $SU(4)$, thus adding to them the identity matrix $i\mathbf{1} = i(\mathbf{1}_A \otimes \mathbf{1}_B)$, we get a basis for the Lie algebra $u(4)$. Any Hermite matrix, after multiplication by the imaginary unit i , can be decomposed in previous basis. In particular, any ρ_u can be rewritten by means of previous basis.

In terms of a basis for a Cartan subalgebra of $iu(n)$, say,

$$\lambda_0 = \begin{vmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{vmatrix}, \quad \lambda_2 = \begin{vmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{vmatrix},$$

$$\lambda_1 = \begin{vmatrix} 1 & & & & \\ & -1 & & & \\ & & 1 & & \\ & & & -1 & \\ & & & & 1 \end{vmatrix}, \quad \lambda_3 = \begin{vmatrix} 1 & & & & \\ & -1 & & & \\ & & -1 & & \\ & & & -1 & \\ & & & & 1 \end{vmatrix}$$

corresponding to $\lambda_0 = \mathbf{1} \otimes \mathbf{1}$, $\lambda_1 = \sigma_3 \otimes \mathbf{1}$, $\lambda_2 = \mathbf{1} \otimes \sigma_3$, $\lambda_3 = \sigma_3 \otimes \sigma_3$.

We may write a generic density state in the form

$$U \frac{1}{4} (\lambda_0 + p^1 \lambda_1 + p^2 \lambda_2 + p^3 \lambda_3) U^\dagger = \frac{1}{4} (\lambda_0 + \vec{p} \vec{\lambda}),$$

where \vec{p} is a vector in the 15-dimensional space and $\vec{\lambda}$ stays for a “vector of matrices” in the 15-dimensional Lie algebra $su(4)$.

In terms of the states of the component systems, we can now express operators as “quadratic functions” and compute the Riemann–Jordan bracket and the Poisson bracket in terms of those of the component systems.

By using evident notation, we may consider “quadratic functions”

$$\langle \psi | \otimes \langle \varphi | A \otimes B | \varphi \rangle \otimes | \psi \rangle = \langle \psi | A | \psi \rangle \otimes \langle \varphi | B | \varphi \rangle,$$

which are really “biquadratic” if we parametrize states in terms of the states of the component systems.

The Poisson bracket is defined by

$$\{f_A \otimes f_B, g_A \otimes g_B\} = \{f_A, g_A\} \otimes f_B g_B + f_A g_A \otimes \{f_B, g_B\},$$

more specifically

$$\{z_m w_n, z_r w_s\} = \{z_m, z_r\} w_n w_s + z_m z_r \{w_n, w_s\}$$

and similarly for the Riemann–Jordan brackets.

8. Conclusions and outlook

In this paper, we have shown how it is possible to provide a geometrical formulation of quantum mechanics in a way that makes possible to use also nonlinear transformations. Not only it seems possible to achieve a great level of geometrization of quantum mechanics comparable to the one obtained in classical mechanics and general relativity but, in addition, elsewhere we will show how to put to work this covariant formulation of quantum mechanics for a full study of composite systems and how to tackle the problem of separability and entanglement.

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