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Typical states and density matrices

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It is shown how, for an n-dimensional Hilbert space, one may translate the density matrix formalism into a sort of classical probability theory on the space of quantum states, $P_{n-1}(\mathbb{C})$. Because of the intricate blend of complex, Riemannian and symplectic geometry which arises from the Kähler structure on this manifold, under this transcription Schrödinger's equation becomes Hamilton's equation and Heisenberg's equation becomes Liouville's equation. The formalism suggests some natural generalizations of conventional quantum mechanics which are briefly described.

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1. Introduction

Roger Penrose has, over the years, frequently emphasized the importance of the complex numbers for quantum mechanics and in particular that the pure states of the simplest quantum system, for example a spin ½ system, make up the points of a complex manifold $P_1(\mathbb{C})$, the complex projective line. This is not only a complex manifold, diffeomorphic to S^2 but a Riemannian manifold as well. One quarter of the standard round metric on S^2 is not only compatible with the complex structure but plays an essential role in quantum mechanics because the probability that a pure state $|\psi_1\rangle$ may be found in a pure state $|\psi_2\rangle$ is given by $|\langle\psi_2|\psi_1\rangle|^2$, where

$$|\langle\psi_2|\psi_1\rangle| = \cos d\,, \tag{1.1}$$

and where d is the distance along the great circle (measured with respect to this rescaled metric) passing through the associated points x_1 and x_2 on the two-sphere. [Because of the rescaling d cannot exceed $\pi/2$ and so the right hand side of (1) is never negative.]

By now it has become well known how this picture changes as one passes to quantum systems with a large, but finite dimensional Hilbert space $\mathscr{H}_n$. Pure states are associated with rays in $\mathscr{H}_n$, i.e. equivalence classes of vectors $|\psi\rangle$ differing by multiplication by a non-vanishing complex number. Choosing a basis $|\psi_i\rangle$, $i=1$, 2, ..., n for $\mathcal{H}_n$ in which the components of a representative state are

$$|\psi\rangle = Z^i |\psi_i\rangle \ , \tag{1.2}$$

we see that pure states correspond to equivalence classes of n-tuples of complex numbers $\{Z^i\}$ such that $\{Z^i\}$ and $\{\lambda Z^i\}$, $\lambda \in \mathbb{C} - \{0\}$, are identified. This is just the standard definition of complex projective $(n-1)$-space $P_{n-1}(\mathbb{C})$. Moreover we may endow $P_{n-1}(\mathbb{C})$ with a Riemannian metric compatible with the complex structure which determines quantum-mechanical transition probabilities in just the same way as it does in the case of $P_1(\mathbb{C})$. In fact since any two pure states $|\psi_1\rangle$ and $|\psi_2\rangle$ may be joined by a complex projective line in $P_{n-1}(\mathbb{C})$ we need only repeat the previous construction and use formula (1.1). The result is called the Fubini–Study metric on $P_{n-1}(\mathbb{C})$.

What appears to be slightly less well known is how to treat a general mixed state from this geometrical point of view. The obvious and correct guess is that one should use a sort of probability distribution on $P_n(\mathbb{C})$. In this article I shall show how this is done. In fact little of what I have to say can be described as new but it is not easy to find a description using the notation and ideas familiar to most physicists – Dirac's bras and kets for quantum mechanics and the standard if somewhat old fashioned index notation used in General Relativity. Another of Roger's persistent, if minor, themes has been the importance of adopting a serviceable, standard and familiar notation which, despite the shifts of mathematical fashion, allows the immediate recognition of the nature, tensorial or otherwise, of the objects one is using.

More substantial reasons for spelling out these ideas are their possible application to quantum cosmology, which first prompted me to work out the details [1], and because, having set up the formalism, it suggests natural generalizations (which I shall only hint at here) taking us beyond conventional quantum mechanics. This again is not a new idea but in view of the intimate relationship between quantum mechanics, Riemannian geometry, Hamiltonian, symplectic and complex geometry which show up here – mainly in the guise of Kähler geometry – it seems worth making the point again.

The restriction to finite dimensional Hilbert spaces does not seem to me to be a serious physical limitation since I find it difficult to believe that there is a physical distinction between using a finite but large dimensional Hilbert space and an infinite dimensional one. Of course mathematically the latter is usually much more convenient despite the fact that it also introduces the familiar problem of ultraviolet divergences of quantum field theories as well as the rather less familiar but, I believe, equally serious infrared divergences that one encounters when attempting to discuss infinitely large universes, as one does in quantum cosmology. In that context one encounters the problem that wave functions of the universe are not normalizable because of their behaviour for large scale factor. In fact there are even reasons for preferring a truly discrete version of quantum mechanics in which the total number of allowed quantum states is finite. In such a theory no divergence should possibly occur. This would take us away from complex Hilbert spaces of course. A different reason for not using complex Hilbert spaces in quantum cosmology is the intimate relation between the complex numbers and the notion of time evolution in quantum mechanics. If the evolution of the wave function is non-unitary, for example, or if the allowed wave functions of the entire universe must all be real because they should not provide a direction of time, or if there is no global notion of time at all, then the need for the complex numbers at a truly fundamental level might be lost.

2. The Fubini–Study metric

The Hilbert space $\mathscr{H}_n$ carries a natural flat Hermitian metric:

$$\langle \mathrm{d}\psi | \mathrm{d}\psi \rangle = \langle \psi_i | \psi_j \rangle \, \mathrm{d}\bar{Z}^{\bar{i}} \mathrm{d}Z^j . \tag{2.1}$$

If the basis $\{ |\psi_i\rangle \}$ is orthonormal this becomes

$$\mathrm{d}\bar{Z}_i \, \mathrm{d}Z^i , \tag{2.2}$$

where I adopt the notation in $\mathbb{C}^n$ that an unbarred index on a barred quantity has been raised or lowered using the flat metric

$$\delta_{\bar{i}j} = \langle \psi_i | \psi_j \rangle . \tag{2.3}$$

Restricted to states of unit norm, $\langle \psi | \psi \rangle = 1$, leads to $\bar{Z}_i Z^i = 1$; this is the canonical unit round metric on S^{2n-1}. We may view S^{2n-1} as a circle bundle over $P_{n-1}(\mathbb{C})$ by associating each normalized bra $|\psi\rangle$ with its equivalence class under $|\psi\rangle \to e^{i\alpha} |\psi\rangle$. This gives us the Hopf fibration. The map, which moves points along the fibres, $|\psi\rangle \to e^{i\alpha}|\psi\rangle$, is an isometry of the round metric and so we may define the distance between two nearby pure states as the perpendicular distance between their associated fibres. Thus, if $|\psi\rangle$ is normalized,

$$|\mathrm{d}\psi\rangle - \frac{1}{2\mathrm{i}} (\langle \psi | \mathrm{d}\psi \rangle - \langle \mathrm{d}\psi | \psi \rangle) |\psi\rangle \tag{2.4}$$

is perpendicular to the fibres and thus the Fubini–Study metric is

$$\langle \mathrm{d}\psi | \mathrm{d}\psi \rangle - \tfrac{1}{4} | \langle \psi | \mathrm{d}\psi \rangle - \langle \mathrm{d}\psi | \psi \rangle |^2 . \tag{2.5}$$

To obtain an explicit expression in terms of local coordinates x^α, $\alpha = 1, 2, \ldots, 2n-2$, on $P_{n-1}(\mathbb{C})$ we pick a local section of the circle bundle over $P_{n-1}(\mathbb{C})$, which means in practical terms parameterizing our normalized states $|\psi\rangle$ as

$$|\psi\rangle = e^{i\beta} |\psi_0(x^\alpha)\rangle ,$$

where the phase of $|\psi_0(x^\alpha)\rangle$ is fixed by some convention. The Fubini–Study metric (2.5) is then easily seen to be independent of the phase β and depends only on the $2n-2$ coordinates x^α. If $g_{\alpha\beta}$ is the metric then

$$g_{\alpha\beta}\,\mathrm{d}x^\alpha\,\mathrm{d}x^\beta=\langle \mathrm{d}\psi_0\,|\,\mathrm{d}\psi_0\rangle-\tfrac{1}{4}|\langle\psi_0\,|\,\mathrm{d}\psi_0\rangle-\langle\mathrm{d}\psi_0\,|\,\psi_0\rangle|^2\,.$$

In what follows we shall not need to use any particular coordinate system on $P_{n-1}(\mathbb{C})$ and our results will be independent of any such choice. For concreteness, however, the reader may have in mind the case $n=2$, which we may parameterize as

$$|\psi\rangle=\mathrm{e}^{\mathrm{i}\beta}\begin{pmatrix}\mathrm{e}^{\mathrm{i}\phi/2}\cos\theta/2\\ \mathrm{e}^{-\mathrm{i}\phi/2}\sin\theta/2\end{pmatrix},$$

where $x^\alpha=(\theta,\phi)$ and (2.5) becomes $\frac{1}{4}(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2)$. This is just $\frac{1}{4}$ the standard round metric on S^2. The case $n=3$ may be found worked out in detail in refs. [2,3]. It is the case that the Fubini–Study metric is Einstein and so the case $n=3$ (spin 1) may also be regarded as a gravitational instanton. It may also be amusing for relativists to note that, since $P_{n-1}(\mathbb{C})$ admits an obvious SU(2) action (acting linearly on Z^1 and Z^2) and an obvious SO(3) action (acting linearly on Z^1, Z^2, Z^3), the Fubini–Study metric may be cast in Bianchi-IX form in two distinct ways: in the former case with 2 invariant directions equal and in the latter case with all 3 invariant directions unequal.

3. Observables and density matrices

A physical observable O is associated with a self-adjoint operator $\hat{O}$ and $\mathcal{H}_n$ and the set of such observables form a real n^2 dimensional vector space if we include the unit observable $\hat{I}$. Such observables determine and are determined by their diagonal matrix elements, which are real-valued functions $O(x^\alpha)$ on $P_{n-1}(\mathbb{C})$. Explicitly

$$O(x)=\langle\psi(x)\,|\,\hat{O}\,|\,\psi(x)\rangle\,. \tag{3.1}$$

Note that not every real-valued function on $P_{n-1}(\mathbb{C})$ is an observable.

Mixed states are associated with density matrices $\hat{\rho}$ which are positive semi-definite observables. Thus they determine a non-negative function $\rho(x)$, which we may interpret as a probability density giving the probability that the system is in the pure state $|\psi(x)\rangle$. We may use $\rho(x)$ to calculate the expectation value O_ρ of any observable $\hat{O}$ in the mixed state $\hat{\rho}$. The usual formula is

$$O_\rho=\mathrm{Tr}(\hat{O}\hat{\rho})/\mathrm{Tr}\,\hat{\rho}\,. \tag{3.2}$$

We shall translate the right hand side of (3.2) into an integral over $P_{n-1}(\mathbb{C})$, using the Gaussian integral

$$\int_{\mathbb{C}^n} d^nY\, d^n\bar{Y}\, (\bar{Y}_i\bar{Y}_j Y^r Y^s) \exp(-|Y|^2) = \pi^n(\delta^r_i\delta^s_j + \delta^r_j\delta^s_i) . \tag{3.3}$$

Equation (3.3) may be obtained by differentiating twice the expression

$$\int_{\mathbb{C}^n} d^nY\, d^n\bar{Y} \exp(-|Y|^2 + \bar{J}_i Y^i + J^k \bar{Y}_k) = \pi^n \exp \bar{J}_i J^i \tag{3.4}$$

with respect to $\bar{J}_i$ and J^k.

If $A^r{}_j$ and $B^s{}_i$ are the components of two self-adjoint operators $\hat{A}$ and $\hat{B}$ in the orthonormal basis $|\psi_i\rangle$ they determine two real-valued functions $A(x)$ and $B(x)$ on $P_{n-1}(\mathbb{C})$ by

$$A(x) = \langle\psi|\hat{A}|\psi\rangle = \bar{Z}_r A^r{}_j Z^j \tag{3.5}$$

and similarly for $\hat{B}$, where Z^j are the components of the normalized ket $|\psi\rangle$. The ket $r|\psi\rangle$ is unnormalized and has components $Y^i = rZ^i$ which range over all of $\mathbb{C}^n$. The volume element on $\mathbb{C}^n$ in (3.3) may be written as

$$d^n\bar{Y}\, d^nY = r^{2n-1}\, dr\, d\Omega_{2n-1} , \tag{3.6}$$

where $d\Omega_{2n-1}$ is the canonical Riemannian volume element on S^{2n-1} with its round metric of unit radius. This latter volume element is related to that on $P_{n-1}(\mathbb{C})$, $\sqrt{g}\, d^{2n-2}x$, by

$$d\Omega_{2n-1} = d\beta \sqrt{g}\, d^{2n-2}x . \tag{3.7}$$

We can now substitute (3.5), (3.6) and (3.7) in (3.3) to obtain the following identity:

$$\mathrm{Tr}\, \hat{A}\hat{B} + \mathrm{Tr}\, \hat{A}\, \mathrm{Tr}\, \hat{B} = \frac{(n+1)!}{\pi^{n-1}} \int_{P_{n-1}(\mathbb{C})} A(x)B(x)\sqrt{g}\, d^{2n-2}x . \tag{3.8}$$

Equation (3.8) contains all the information we need to translate the standard formalism into Riemannian geometric language on $P_{n-1}(\mathbb{C})$. Setting $\hat{A} = \hat{B} = \hat{I}$ the left hand side becomes $n + n^2$. The result is a formula for the volume V of $P_{n-1}(\mathbb{C})$ with its Fubini–Study metric:

$$V = \pi^{n-1}/(n-1)! . \tag{3.9}$$

If $n=2$ we have $V=\pi$; if $n=3$, $V=\pi^2/2$. If $\hat{B}=\hat{I}$ we obtain

$$\mathrm{Tr}\, \hat{A} = \frac{n!}{\pi^{n-1}} \int_{P_{n-1}(\mathbb{C})} A(x)\sqrt{g}\, d^{2n-2}x . \tag{3.10}$$

Consider now a normalized density matrix $\hat{\rho}$,

$$\mathrm{Tr}\, \hat{\rho} = 1 . \tag{3.11}$$

The expectation value of an observable $\hat{O}$ in the state $\hat{\rho}$ is given by

$$O_\rho = \frac{(n+1)!}{\pi^{n-1}} \int_{P_{n-1}(\mathbb{C})} \left(\rho(x) - \frac{1}{(n+1)}\right) O(x)\sqrt{g}\, \mathrm{d}^{2n-2}x \,. \qquad (3.12)$$

We may interpret (3.12) as meaning that a density matrix $\rho(x)$ corresponds to a sort of probability density $P(x)$ on $P_{n-1}(\mathbb{C})$ given by

$$P(x) = \frac{n(n+1)}{V}\left(\rho(x) - \frac{1}{(n+1)}\right). \qquad (3.13)$$

In the special case that $\hat{\rho} = (1/n)\hat{I}$, the totally mixed state of local ignorance in which no particular pure state is favoured, we found

$$P = 1/V \,, \qquad (3.14)$$

and thus points on $P_{n-1}(\mathbb{C})$ are populated with equal probability in this state. In ref. [1] such states were referred to as "typical". Note that the second term in (3.9) may be discarded if we only consider observables $\hat{O}$ which are trace free, i.e., which are orthogonal in the metric $\mathrm{Tr}(\hat{O}_1\hat{O}_2)$. If we do not make this restriction we find that the probability densities given by (3.13) need not be everywhere positive, though $\rho(x)$ always is. In fact, the probability density $P(x)$ is to some extent ill defined since the set of observables is finite dimensional and spanned by n_2 operators $\hat{\pi}_{ij}$,

$$\hat{\pi}_{ij} = \tfrac{1}{2}(|\psi_i\rangle\langle\psi_j| + |\psi_j\rangle\langle\psi_i|) \,,$$

determining n^2 functions $\pi_{ij}(x)$ on $P_{n-1}(\mathbb{C})$. We could add to the right hand side of (3.13) any function $f(x)$ on $P_{n-1}(\mathbb{C})$ which is orthogonal to the π_{ij}'s, i.e., which satisfies

$$\int_{P_{n-1}(\mathbb{C})} f(x)\pi_{ij}(x)\sqrt{g}\, \mathrm{d}^{2n-2}x = 0 \,, \quad i = 1, 2, \ldots, n \,.$$

Another unusual feature of the probability distribution is of course that, even if we know for certain that the system is in a particular state $|\psi_1\rangle$ say, the associated probability distribution $\pi_1(x)$ is non-zero almost everywhere on $P_{n-1}(\mathbb{C})$; it vanishes only on states which are orthogonal to $|\psi_1\rangle$, which is a submanifold of co-dimension 2, isomorphic to $P_{n-2}(\mathbb{C})$.

4. Poisson structure and evolution

The set of observables, $\{\hat{O}\}$, may be thought of as a subspace of the set of all functions on $P_{n-1}(\mathbb{C})$, spanned, for example, by the n^2 functions

$$\pi_{ij} = \langle\psi|\hat{\pi}_{ij}|\psi\rangle \qquad (4.1)$$

with

$$\hat{\pi}_{ij} = \tfrac{1}{2}(|\psi_i\rangle\langle\psi_j| + |\psi_j\rangle\langle\psi_i|) = \hat{\pi}_{ji} . \tag{4.2}$$

More geometrically we may think of the observables as the direct sum of the constant function and the lowest non-trivial eigenspace of the Laplacian acting on scalars associated to the Fubini–Study metric on $P_{n-1}(\mathbb{C})$. We may endow $\{\hat{O}\}$ with two important algebraic structures. The first is the commutative Jordan product

$$(\hat{A}, \hat{B}) \to \hat{A}\bullet\hat{B} = \hat{B}\bullet\hat{A} = \tfrac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A}) . \tag{4.3}$$

The second is the anticommutative Lie product or commutator

$$(\hat{A}, \hat{B}) \to \frac{1}{\mathrm{i}}[\hat{A}, \hat{B}] = \frac{1}{\mathrm{i}}(\hat{A}\hat{B} - \hat{B}\hat{A}) . \tag{4.4}$$

The latter product is the more interesting one here since it may be extended to all functions on $P_{n-1}(\mathbb{C})$, not just the observables, and it endows $P_{n-1}(\mathbb{C})$ with a Poisson structure which is compatible with its complex and metric structure, the result being that $P_{n-1}(\mathbb{C})$ is a Kähler manifold. The general picture is rather well known. What I want to discuss in detail here is how it applies to the time evolution of both pure states and mixed states. The main point is that we may interpret the Schrödinger equation,

$$\mathrm{i}\, \mathrm{d}|\psi\rangle/\mathrm{d}t = \hat{H}|\psi\rangle , \tag{4.5}$$

as Hamilton's equations on $P_{n-1}(\mathbb{C})$ with Hamiltonian function

$$H(x) = \langle\psi(x)|\hat{H}|\psi(x)\rangle , \tag{4.6}$$

and the Heisenberg equation of motion for a general density matrix,

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \frac{1}{\mathrm{i}}[\hat{\rho}, \hat{H}] , \tag{4.7}$$

becomes the Liouville equation

$$\mathrm{d}\rho/\mathrm{d}t = \{\rho, H\} , \tag{4.8}$$

where $\{\ ,\ \}$ is the Poisson bracket. Thus from a purely formal point of view, setting aside questions of interpretation, the quantum and classical theories may be cast into an identical form!

The easiest route to these results is the symplectic quotient construction of Marsden and Weinstein extended to the Kähler case (see, e.g., ref. [4]). The flat metric on $\mathbb{C}^n$ given by (2.1),

$$\mathrm{d}s^2 = \mathrm{d}\bar{Y}^m\, \mathrm{d}Y^n\, \delta_{mn} , \tag{4.9}$$

is manifestly Kähler, i.e.,

$$ds^2 = \frac{\partial^2 K}{\partial \bar{Y}^m \, \partial Y^n} \, d\bar{Y}^m \, dY^n \,, \tag{4.10}$$

with Kähler potential

$$K(\bar{Y}, Y) = \bar{Y}_m Y^m \tag{4.11}$$

and symplectic form

$$\omega = \tfrac{1}{2}\mathrm{i} \, dY^m \wedge d\bar{Y}_m \,. \tag{4.12}$$

We may therefore define the Poisson bracket of two real-valued functions F and G by

$$\{F, G\} = \mathrm{i}\left(\frac{\partial F}{\partial \bar{Y}_m}\frac{\partial G}{\partial Y^m} - \frac{\partial F}{\partial Y^m}\frac{\partial G}{\partial \bar{Y}_m}\right). \tag{4.13}$$

Now the holomorphic map

$$Y^m \to e^{\mathrm{i}\alpha} Y^m \tag{4.14}$$

is both an isometry of the flat metric and a canonical transformation with respect to the Poisson structure given by (4.13). It is generated by the function

$$\Theta = -\bar{Y}_m Y^m \,, \tag{4.15}$$

since (4.14) corresponds to moving along the integral curves of the equation

$$dY^i/d\alpha = \mathrm{i}Y^i = \{Y^i, \Theta\} \,. \tag{4.16}$$

The Marsden–Weinstein construction in the present case consists of restricting attention to a level set of the moment map Θ, e.g.,

$$\Theta = -1 \,, \tag{4.17}$$

and identifying points under the U(1) action (4.14). If F and G are two functions invariant under (4.14) (which is of course just the Hopf map we used earlier) we may consider them as functions on $P_{n-1}(\mathbb{C})$, by restricting them to the level set given by (4.17), and take the Poisson bracket to be given by the restriction of (4.13). Since the action is both holomorphic and isometric it is not difficult to check that the resulting structure obtained on $P_{n-1}(\mathbb{C})$ is also Kähler.

In the particular case that F and G arise from self-adjoint operators $\hat{F}$ and $\hat{G}$ on H_n in the manner given by (3.5), i.e.,

$$F = \bar{Y}_m F^m{}_s Y^s \,, \tag{4.18}$$

$$G = \bar{Y}_m G^m{}_s Y^s \,, \tag{4.19}$$

one sees from (4.13) that

$$\mathrm{i}\{F, G\} = \langle \psi | \, [\hat{F}, \hat{G}] \, | \psi \rangle \,. \tag{4.20}$$

Equation (4.20) demonstrates the isomorphism between the Poisson algebra of observables on $P_{n-1}(\mathbb{C})$ and the Lie algebra of self-adjoint operators on $\mathscr{H}_n$.

Taking the expectation value of the Heisenberg equation (4.7) now immediately yields [on use of (4.2)], the Liouville equation (4.8). To obtain the Hamilton equation on $P_{n-1}(\mathbb{C})$,

$$\mathrm{d}x^\alpha/\mathrm{d}t=\{x^\alpha, H\}\ , \tag{4.21}$$

from the Schrödinger equation (4.5) we expand (4.5) in a basis to yield

$$\mathrm{i}\,\mathrm{d}Y^m/\mathrm{d}t=H^m{}_sY^s\ , \tag{4.22}$$

where $H^m{}_s$ are the matrix elements of $\hat{H}$ in an orthonormal basis,

$$H^m{}_s=\langle\psi_m|\hat{H}|\psi_s\rangle\ . \tag{4.23}$$

Using the definition of the Poisson bracket (4.13) we may rewrite (4.22) as

$$\mathrm{d}Y^m/\mathrm{d}t=\{Y^m, H\}\ . \tag{4.24}$$

Equation (4.24) is in Hamiltonian form. It preserves the normalization condition (4.17) and commutes with the Hopf fibration and so it may pushed down to $P_{n-1}(\mathbb{C})$ yielding (4.21).

The Hamiltonian vector field H^α associated to the Hamiltonian function H,

$$H^\alpha=\omega^{\alpha\beta}\,\partial H/\partial x^\beta\ , \tag{4.25}$$

is a holomorphic Killing vector field of the Fubini–Study metric $g_{\alpha\beta}$ and hence it generates an isometry of this metric [in fact a one-parameter subgroup of $SU(n)/\mathbb{Z}_n$]. This guarantees that the transition probability given by (1.1) remains constant in time, since the distance d between two pure states $|\psi_1\rangle$ and $|\psi_2\rangle$ evolved with the same Hamiltonian $H(x)$ must remain constant since isometries preserve the Riemannian volume element $\sqrt{g}\,\mathrm{d}^{2n-2}x$ or equivalently $\omega^n/n!$, where ω is the symplectic two-form. The Hamiltonian flow generated by the function $H(x)$ of the form (4.6) will preserve the expectation values given by (3.12) and evolved using Liouville's equation (4.8).

The fact that the isometries of $P_{n-1}(\mathbb{C})$ with its Fubini–Study metric can be lifted to $\mathbb{C}^n$ as unitary or anti-unitary transformations is known to physicists as Wigner's Theorem. These isometries will, in general, have fixed points. In the case of Hamilton's equations the fixed points are called stationary states and correspond to critical points of the Hamiltonian, i.e., points for which

$$\partial H/\partial x^\alpha=0\ . \tag{4.26}$$

This statement is just the variational principle for the energy eigenvalues E_k, $k=1, 2, \ldots, n$. In the case that the eigenvalues are all distinct we can list them in increasing order $E_1<E_2<\cdots<E_n$. The Morse index p of the critical point associated to E_k is easily seen to be $2(n-k)$ and so using H as a Morse function we can calcu-

late the Euler number χ of $P_{n-1}(\mathbb{C})$ as

$$\chi = \sum_{p=0}^{2n-2} n_p(-1)^p = \sum_{k=1}^{n} (-1)^{2(n-k)} = n\,, \tag{4.27}$$

where n_p is the number of critical points of Morse index p.

The Hamiltonian as opposed to the complex or Riemannian geometry of the space of pure states is not as well known as it might be. It is, however, sometimes used without people realizing the fact. An example of this is provided by the Holstein–Primakoff transformation often used to discuss spin systems. Roughly speaking this corresponds to using a Darboux or canonical coordinate system for S^2 rather than a complex coordinate system. Cartographically speaking the distinction is that between Lambert's "Polar Zenithal Equal Area projection" and the more usual stereographic "Polar Zenithal Equal Angle projection". Since a full exposition is slightly involved I shall defer a detailed consideration to some other occasion.

5. Time and the complex numbers

Much of the basis structure of quantum mechanics is projective geometry, augmented with an appropriate metric with which to construct transition probabilities. As such it could be over almost any field. In particular one could, and people do, imagine quantum mechanics over $\mathbb{R}$, the real numbers, $\mathbb{C}$, the complex numbers, and $\mathbb{H}$, the quaternions. A more novel idea is to consider discrete quantum mechanics over a finite field, for example, a Galois field of characteristic p. This would have the consequence that a finite dimensional quantum system, i.e., one with a finite dimensional Hilbert space, would have a finite number of quantum states rather than an infinite number, as for example with $P_{n-1}(\mathbb{C})$, which seems more intuitively appealing. A problem with discrete quantum mechanics is, however, the introduction of real-valued probabilities, which presumably only emerge in the limit that the characteristic p tends to infinity.

The choice of field is closely related to the concept of time. A discrete field presumably entails a discrete time variable. On the other hand, a real field seems to allow no time evolution at all. The real projective spaces $P_{n-1}(\mathbb{R})$ have a metric structure but no symplectic structure, compatible with the metric. If they did they would have an almost complex structure, but since $P_{n-1}(\mathbb{R}) = S^{n-1}/\pm 1$ and the only spheres to admit an almost complex structure are S^2 and S^6, neither of which descends to $P_{n-1}(\mathbb{R})$, we are led to a contradiction.

In fact, real quantum mechanics usually arises when one considers time-reversal invariant systems. In Hamiltonian mechanics a time-reversing transformation is anticanonical or antisymplectic: it reverses the sign of the symplectic form. In conventional quantum mechanics time reversal is effected by an antiholomorphic isometry on $P_{n-1}(\mathbb{C})$, which lifts to an anti-unitary map on $\mathcal{H}_n$. Thus the two concepts agree for the case of Kähler geometry. Time reversal is usually thought of as an involution of order 2 on the space of quantum states. If it lifts to an involution of order 2 on $\mathcal{H}_n$ one may, by appropriate choice of basis, regard it as complex conjugation of the homogeneous complex coordinates Z^i. If the Hamiltonian is invariant under time reversal then the critical points or stationary states may be taken to lie in the real projective subspace $P_{n-1}(\mathbb{R})$. In an appropriate basis the Hamiltonian is real and symmetric. Thus, in the familiar spin $\frac{1}{2}$ example, if

$$\hat{H}=\mu \boldsymbol{B}\cdot\boldsymbol{\sigma}\,, \tag{5.1}$$

where $\boldsymbol{B}=(0, 0, B)$ and σ_i are the Pauli matrices, the two stationary states are $|\psi_\uparrow\rangle=\binom{1}{0}$ and $|\psi_\downarrow\rangle=\binom{0}{1}$ and in this basis

$$\hat{H}=\begin{pmatrix}\mu B & 0\\ 0 & -\mu B\end{pmatrix}. \tag{5.2}$$

We have that $P_1(\mathbb{R})$ is the meridian $\phi=0$. The Hamiltonian flow generated by (5.1) is along the small circles of fixed latitude. The only trajectories to lie in this real subspace are the stationary states themselves; in other words, the only real states are stationary states. These are also the only states which are strictly time-reversal invariant for all time in the sense that

$$|\psi(t)\rangle^*=\lambda|\psi(t)\rangle \tag{5.3}$$

for some $\lambda\in\mathbb{C}-\{0\}$.

On the other hand, we might demand that the evolution backwards in time is the same as forwards in time:

$$|\psi(t)\rangle^*=\nu|\psi(-t)\rangle \tag{5.4}$$

for some $\nu\in\mathbb{C}-\{0\}$. If

$$|\psi(t)\rangle=\begin{pmatrix}a\mathrm{e}^{-\mathrm{i}\omega t}\\ b\mathrm{e}^{+\mathrm{i}\omega t}\end{pmatrix} \tag{5.5}$$

with $\omega=\mu B$, we can satisfy (5.4) by setting $a\bar{b}=b\bar{a}$. The set of such allowed states are precisely those lying on the meridian $\phi=0$, in other words, it is parameterized by the real projective line $P_1(\mathbb{R})$.

The situation described above generalizes for all n provided the time-reversing involution of order 2 on $P_{n-1}(\mathbb{C})$ lifts to an anti-unitary involution of order 2 on $\mathcal{H}_n$. Thus, for example, for a spin 1 system with time-reversal invariant Hamiltonian the time-reversal invariant states in the sense of (5.4) are parameterized by points on the real projective plane, $P_2(\mathbb{R})$. It may happen that the time-reversing involution on $P_{n-1}(\mathbb{R})$ that commutes with the Hamiltonian lifts to an involution of order 4 on $\mathcal{H}_n$. The result is quaternionic quantum mechanics. This situation is most frequently encountered when dealing with systems with odd spin s. Since the theory involves two-component SU(2) spinors $\Psi^{AB\ldots G}$ with $2s=n-1$ totally symmetric indices, it is perhaps worth recalling in detail on this festive occasion. The SU(2) invariant metric $\delta_{A'B}$ and the symplectic form ϵ^{AB} allow one to construct an SU(2)-invariant map J from $\mathscr{H}_n$ to its complex conjugate space $\bar{H}_n$ using the SU(2)-invariant tensor

$$J^A_{A'}=\epsilon^{AC}\delta_{A'C}\,. \tag{5.6}$$

The crucial property of $J^A_{A'}$ is that

$$J^A_{A'}\bar{J}^{A'}_B=-\delta^A_B\,, \tag{5.7}$$

where $\bar{J}^{A'}_B$ is the complex conjugate of $J^A_{B'}$ and δ^A_B is the Kronecker delta.

We may now associate, in an SU(2)-invariant way, with every SU(2) spinor $\Psi^{AB\ldots FG}$ its time-reversed spinor

$$(J\Psi)^{AB\ldots FG}=J^A_{A'}J^B_{B'}\cdots J^G_{G'}\bar{\Psi}^{A'B'\ldots G'}\,, \tag{5.8}$$

where $\bar{\Psi}^{A'B'\ldots G'}$ is the complex conjugate of $\Psi^{AB\ldots G}$. If the spin $s=\frac{1}{2}(n-1)$ is a half integer, that is, if the number of indices on the spinor $\Psi^{AB\ldots G}$ is odd, the map defined by (5.8) is, because of (5.6), of order 4. In fact, regarding $\mathscr{H}_{2k}$ as $\mathbb{R}^{4k}$, J is a real linear map satisfying

$$J^2=-\mathrm{id}\,. \tag{5.9}$$

Moreover multiplication by the square root of -1 may also be regarded as a real linear map on $\mathbb{R}^{4k}$, which we represent as I. Clearly

$$I^2=-\mathrm{id}\,. \tag{5.10}$$

Because the action of J involves complex conjugation, the action of I and J anticommute:

$$IJ=-JI\,. \tag{5.11}$$

If we define a third real linear map K on $\mathbb{R}^{4k}$ by

$$IJ=K\,, \tag{5.12}$$

it follows from (5.9), (5.10) and (5.11) that

$$K^2=-\mathrm{id}\,, \tag{5.13}$$

$$JK=I=-KJ\,, \tag{5.14}$$

$$KI=J=-IK\,. \tag{5.15}$$

Thus we have an action of the quaternions $\mathbb{H}$ on $\mathbb{R}^{4k}$, and we may regard $\mathscr{H}_{2k}$ as a quaternionic vector space and the Hamiltonians which are are invariant under time reversal defined by (5.8) (and which are rotationally invariant) may be regarded as quaternion-valued Hermitian matrices.

It is not possible to find states which are equal to their time-reversed state if one uses (5.8), because of (5.9). The proper analogue of complex conjugation is now quaternionic conjugation. The states which are proportional to their quaternionic conjugate lie in a real $(k-1)$ dimensional projective subspace $P_{k-1}(\mathbb{R}) \subset P_{2k-1}(\mathbb{C})$. The lowest non-trivial case is $k=2$, $n=4$ or spin $s=\frac{3}{2}$.

A quantum cosmological application of these ideas (at least in the simpler case when time evolution is represented by complex conjugation) arises when one tries to quantize quantum fields in spacetimes, like for example the Schwarzschild or De Sitter spacetimes, in which spacetime events related by a time-reversing isometry of the spacetime metric are identified (the so called "elliptic" interpretation). One way of expressing the difficulties one encounters is to say that one is forced to adopt a real quantum-mechanical Hilbert space [5]. It is possible that the more complicated situation involving the quaternions might arise if one was to consider fermions in quantum cosmology as one must, for example, if one is considering supergravity theories.

6. Generalizations

The basic set up described above admits some obvious generalizations, some of which have certainly already been proposed in the literature. Roughly speaking they may be classified into conservative and radical:

In the *conservative case*, $P_{n-1}(\mathbb{C})$ is retained as the state space and merely the dynamics is altered so that the evolution is non-linear and non-unitary whether it operates on pure states (as in the proposal of Kibble [6], for example) or on density matrices (as in the proposal of Hawking [7]).

In the *radical case*, $P_{n-1}(\mathbb{C})$ is abandoned and a different state space, $P_{n-1}(\mathbb{R})$ or $P_{n-1}(\mathbb{H})$, is considered as in real or quaternionic quantum mechanics, or even more radically the underlying linear structure of projective geometry is abandoned altogether and $P_{n-1}(\mathbb{C})$ is replaced by a more general class of Kähler manifolds.

I must admit I find the radical proposal by far the more attractive but it seems to encounter a number of difficulties. These relate to questions such as what is an appropriate choice of observables? The lowest non-trivial eigenspace of the Laplacian, for example, would in general be just one dimensional and even if it were not it is not likely to generate holomorphic isometries. Another difficulty is how to treat composite systems. Rather than pursue this theme *in extenso* I will close by making a few unsystematic remarks about possible generalizations of this sort. My main aim, however, in this article was to explain how to incorporate mixed states in the conventional picture in a perhaps slightly unconventional but I hope useful way.

7. Superscattering operators

One generalization of conventional quantum mechanics is to replace unitary time evolution, which takes pure states to pure states, by an evolution law which can take pure states to mixed states. This may arise as an approximation to some underlying and more complicated unitary evolution (as in irreversible thermodynamics) or may be taken as a fundamental modification of quantum mechanics forced on us by quantum gravitational effects associated with event horizons for example. In both approaches one invokes the action of a linear map $, which takes density matrices to density matrices and which leaves invariant the unit density matrix,

$$\$\hat{I}=\hat{I}\,. \tag{7.1}$$

The infinitesimal form of this evolution is a master equation, which may be written on $P_{n-1}(\mathbb{C})$ as

$$\mathrm{d}\rho/\mathrm{d}t=M\rho\,, \tag{7.2}$$

where the vector field $M^\alpha\,\partial/\partial x^\alpha$ must preserve phase space volume, i.e., be divergence free,

$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial x^\alpha}(\sqrt{g}\,M^\alpha)=0\,. \tag{7.3}$$

Page [8] and Wald [9] have pointed out, in the quantum gravity context, and other people more generally, that demanding strict time reversibility leads to the result that the evolution must in fact be unitary. In the present context this means that the vector field M^α in (7.2) must be a holomorphic Killing vector of the Fubini–Study metric. It would be interesting to understand this result in a more geometrical way. The natural way to go about this would be to consider how the pure states form the boundary of the convex set of mixed states. Geometrically this is related to the Veronese embedding of projective spaces.

8. Composite systems

Some of the most mysterious features of quantum mechanics arise when one considers composite systems obtained by combining two systems with Hilbert space $\mathcal{H}_n$ and $\mathcal{H}_m$ of dimension n and m, respectively. The combined Hilbert space is taken as the tensor product $\mathcal{H}_n\times\mathcal{H}_m$ and the associated space of states is $P_{nm-1}(\mathbb{C})$, which has a much larger dimension than that of the cartesian product $P_{n-1}(\mathbb{C})\times P_{m-1}(\mathbb{C})$ of the two individual state spaces, which has only dimension $n+m-2$. The missing information is of course contained in the $(n-1)(m-1)$ relative phases, which have no analogue in the combination of two purely classical phase spaces.

The fact that products of projective spaces admit an embedding of this sort, called by algebraic geometers the Segre embedding, seems to be very special. If one wished to generalize quantum mechanics by passing to more general compact Kähler manifolds, for example, one would, if one wished to consider composite systems, need some analogue of the Segre embedding.

A related but rather simpler problem arises if one wishes to generalize the idea of the "Berry phase", i.e., to consider a circle bundle over one space of states which carries information about the overall phase of the system, which is irrelevant for an isolated system but which comes into play when one couples the system to some part of its environment. One might require that the Kähler form serve as the curvature of the line bundle, which will impose integrality conditions on the Kähler form making the manifold one of Hodge type. It then follows from a celebrated theorem of Kodaira that the Kähler manifold admits an embedding into some projective space. Since the result from this embedding is algebraic this might be taken to suggest that passing to a compact Hodge manifold is like considering a constrained set of conventional quantum states.

9. Second quantization

Since the space of states may be viewed as a classical phase space one might ask what happens if one proceeds to quantize this classical phase space using the ideas of geometric quantization. In general this will lead to a different, but still finite dimensional, quantum-mechanical Hilbert space. These Hilbert spaces will carry representations of $U(n)$. By choosing the fundamental representation one has the situation where second quantization yields the first quantized Hilbert space. If one does not make that choice one has the possibility of:

10. Third quantization

and so on.

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