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Geometric quantum mechanics

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Abstract

The manifold of pure quantum states can be regarded as a complex projective space endowed with the unitary-invariant Fubini–Study metric. According to the principles of geometric quantum mechanics, the physical characteristics of a given quantum system can be represented by geometrical features that are preferentially identified in this complex manifold. Here we construct a number of examples of such features as they arise in the state spaces for spin $\frac{1}{2}$, spin 1, spin $\frac{3}{2}$ and spin 2 systems, and for pairs of spin $\frac{1}{2}$ systems. A study is then undertaken on the geometry of entangled states. A locally invariant measure is assigned to the degree of entanglement of a given state for a general multi-particle system, and the properties of this measure are analysed for the entangled states of a pair of spin $\frac{1}{2}$ particles. With the specification of a quantum Hamiltonian, the resulting Schrödinger trajectories induce an isometry of the Fubini–Study manifold, and hence also an isometry of each of the energy surfaces generated by level values of the expectation of the Hamiltonian. For a generic quantum evolution, the corresponding Killing trajectory is quasiergodic on a toroidal subspace of the energy surface through the initial state. When a dynamical trajectory is lifted orthogonally to Hilbert space, it induces a geometric phase shift on the wave function. The uncertainty of an observable in a given state is the length of the gradient vector of the level surface of the expectation of the observable in that state, a fact that allows us to calculate higher order corrections to the Heisenberg relations. A general mixed state is determined by a probability density function on the state space, for which the associated first moment is the density matrix. The advantage of a general state is in its applicability in various attempts to go beyond the standard quantum theory, some of which admit a natural phase-space characterisation.

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1. Introduction

The line of investigation which we refer to as 'Geometric Quantum Mechanics' was inspired in part by the work of Kibble [55,56], who, in a remarkable set of papers, showed how quantum theory could be formulated in the language of Hamiltonian phase-space dynamics. Previously it was generally believed by physicists that it was only *classical* mechanics that exhibited a natural Hamiltonian phase-space structure, to which one had to apply a suitable *quantisation procedure* to produce a very different kind of structure, namely, the complex Hilbert space of quantum mechanics together with a family of linear operators, corresponding to physical observables. However, with the development of geometric quantum mechanics it has become difficult to sustain this point of view, and quantum theory has come to be recognised more as a self-contained entity.

A notable attempt to codify the quantisation procedure in a rigourous mathematical framework was pursued in the *geometric quantisation program* of Kostant, Souriau and others (see, e.g., [99], and references cited therein). Geometric quantum mechanics, however, is not concerned with the quantisation procedure, as such, but accepts quantum theory as given. Indeed, from a modern perspective the nature of the problem has to some extent been reversed, and the main objective now is to understand better how the classical world emerges from quantum theory. Thus, in contrast to the aforementioned 'geometric quantisation' program, what we really need might be more appropriately called a 'geometric classicalisation' program.

To this extent, there may even be grounds for arguing that the notion of quantisation is superfluous. Present thinking on these issues is based on a special relationship between classical and quantum mechanics distinct from the quantisation idea. The key point is that quantum theory possesses an intrinsic mathematical structure equivalent to that of Hamiltonian phase-space dynamics, only the underlying phase space is not that of classical mechanics, but rather the quantum mechanical state space itself, i.e., what we call the 'space of pure states'.

The approach to quantum mechanics achieved via its natural phase-space geometry offers insights into many of the more enigmatic aspects of the theory: linear superposition of states, quantum entanglement, quantum probability, uncertainty relations, geometric phases, and the collapse of the wave function. One of the goals of this paper is to illustrate in geometrical terms the interplay between these aspects of quantum theory.

The plan of the paper is as follows. In Sections 2–4, we introduce a projective geometric framework for quantum mechanics, and review the main features of the quantum phase space. In Section 5, the phase space of a spin 1 system is studied, and in Section 6, we look at a spin $\frac{3}{2}$ system, relating the properties of this system to the geometry of the twisted cubic curve in CP^3. In Section 7, we examine the state space of a spin 2 system, which can be characterised by the specification of a self-conjugate rational quartic curve in CP^4.

In Section 8, we develop a geometric theory of entangled states and discuss the properties of quantum measurements made on such systems, a topic currently of great interest in quantum physics. This theory is extended in Sections 9 and 10, where we introduce a locally invariant geometric measure of entanglement, and explore its applications.

In Sections 11–14, we consider quantum dynamics from a geometric point of view, and demonstrate in particular a quasiergodic property satisfied by the Schrödinger trajectories. We carry out an analysis of the energy surfaces in which the Schrödinger trajectories are confined. We also show that the theory of the geometric phase has a natural characterisation in the present setting, allowing us to introduce a quantum mechanical analogue of the Poincare integral invariant.

Then in Section 15, we examine the status of mixed states in the geometric framework, and discuss the properties of general states characterised by density functions on the quantum phase space. The entropy associated with a general quantum state is shown to be preserved, even under nonlinear dynamics of the Kibble–Weinberg type.

The study of the geometry of the state space of quantum theory has had a rich and lengthy history, including, e.g., the important investigations of von Neumann [94] and Segal [82]. We mention also the influential work of Mielnik [61–63] and Chernoff and Marsden [31]. In addition to Kibble and his collaborators, many other authors (see, e.g., [1,3–5,8,10–12,17–30,32–35,40,42–44,48,51,52,60,77,81,89–93]) have contributed to the development of geometric quantum mechanics, and in doing so have demonstrated that this methodology not only provides new insights into the workings of the quantum world as we presently understand it, but also acts as a base from which extensions of standard quantum theory can be developed, some of which we shall touch upon briefly towards the end of this paper, in Section 16.

2. Projective state space

Let us begin by reviewing briefly how quantum mechanics is ordinarily formulated. A physical system is represented by a wave function $\psi(\mathbf{x}, t)$, which for each time t belongs to a complex Hilbert space $\mathcal{H}$. We also require a set of linear operators on $\mathcal{H}$, corresponding to observables. The wave function characterises the 'state' of the system at time t. In the case of a single particle of mass m moving in Euclidean three-space $\mathbb{R}^3$ under the influence of a potential $\phi(\mathbf{x})$, the evolution of the system is given by Schrödinger's wave equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\mathbf{x}, t) = \left(-\frac{1}{2m}\nabla^2 + \phi(\mathbf{x})\right)\psi(\mathbf{x}, t).$$

Given an initial condition $\psi(\mathbf{x}, 0)$, the Schrödinger equation determines the development of the state, in terms of which we can then calculate the expectation of any observable.

Physical properties of the system depend on the wave function only up to an overall complex factor. Suppose, for instance, we consider an observation to determine whether the particle lies in a region D in $\mathbb{R}^3$. We define the linear operator $\widehat{\chi}_D$, the *characteristic function* for D, by the property $\widehat{\chi}_D\psi(\mathbf{x}) = \psi(\mathbf{x})$ for $\mathbf{x} \in D$ and $\widehat{\chi}_D\psi(\mathbf{x}) = 0$ for $\mathbf{x} \notin D$. Thus $\widehat{\chi}_D$ 'truncates' the wave function outside D. In particular, $\widehat{\chi}_D$ has two eigenvalues, 1 and 0, corresponding to eigenfunctions concentrated on D and on the complement of D in $\mathbb{R}^3$. The probability of an affirmative result for a measurement to determine whether the particle lies in D is given by the expectation of the operator $\widehat{\chi}_D$, i.e.,

$$E[\widehat{\chi}_D] = \frac{\int_{\mathbb{R}^3} \bar{\psi}(\mathbf{x})\widehat{\chi}_D\psi(\mathbf{x})\,\mathrm{d}^3\mathbf{x}}{\int_{\mathbb{R}^3} \bar{\psi}(\mathbf{x})\psi(\mathbf{x})\,\mathrm{d}^3\mathbf{x}}.$$

In this case, we note that the probability density function

$$p(\mathbf{x}) = \frac{\bar{\psi}(\mathbf{x})\psi(\mathbf{x})}{\int_{\mathbb{R}^3} \bar{\psi}(\mathbf{x})\psi(\mathbf{x})\,\mathrm{d}^3\mathbf{x}}$$

on $\mathbb{R}^3$ is independent of the phase and scale of $\psi(\mathbf{x})$. In other words, the state of the system is not given by $\psi(\mathbf{x})$ itself, but rather by an equivalence class modulo transformations of the form

$$\psi(\mathbf{x}, t) \to \Lambda(t)\psi(\mathbf{x}, t)$$

for any nonvanishing complex time-dependent function $\Lambda(t)$. For this reason, we say the state is given, at any time, by a 'ray' through the origin in $\mathcal{H}$. The space of such rays is called projective Hilbert space, denoted $\mathcal{P}H$. Most of the standard operations of quantum mechanics can be referred to $\mathcal{P}H$ directly, without consideration of $\mathcal{H}$ itself. For example, the Schrödinger equation is not invariant under a change of phase and scale for $\psi(\mathbf{x})$, whereas the *projective* Schrödinger equation

$$\mathrm{i}\hbar\left[\psi(\mathbf{y})\frac{\partial\psi(\mathbf{x})}{\partial t} - \psi(\mathbf{x})\frac{\partial\psi(\mathbf{y})}{\partial t}\right] = -\frac{1}{2m}[\psi(\mathbf{y})\nabla^2\psi(\mathbf{x}) - \psi(\mathbf{x})\nabla^2\psi(\mathbf{y})] + [\phi(\mathbf{x}) - \phi(\mathbf{y})]\psi(\mathbf{x})\psi(\mathbf{y})$$

is, in fact, invariant under such transformations, as one can easily verify. Had Schrödinger elected to present this relation as his wave equation, none of the physical consequences would have differed.

3. Pure states

There is a beautiful geometry associated with the projective Hilbert space $\mathcal{P}H$ which is so compelling in its richness that, in our opinion, all physicists should become acquainted with it. The basic idea can be sketched as follows. For simplicity we use an index notation for the Hilbert space $\mathcal{H}$. Instead of $\psi(\mathbf{x})$ we write ψ^α, where the Greek index α labels components of the Hilbert-space vector with respect to a basis. This notation serves us equally well whether $\mathcal{H}$ is finite- or infinite-dimensional (cf. [69,70]). The highly effective use of the index notation for Hilbert space was popularised by Geroch [41]. For the complex conjugate of ψ^α we write $\bar{\psi}_\alpha$. The 'downstairs' index reminds us that $\bar{\psi}_\alpha$ is a 'bra' vector, i.e., it belongs to the dual of the vector space to which ψ^α belongs.

The usual inner product between ψ^α and $\bar{\psi}_\alpha$ can be written $\bar{\psi}_\alpha\psi^\alpha$, with an implied summation over the repeated index. In the case of a wave function, this is equivalent to $\int_{\mathbb{R}^3} \bar{\psi}(\mathbf{x})\psi(\mathbf{x})\,\mathrm{d}^3\mathbf{x}$, which in the Dirac bra–ket notation is $\langle\bar{\psi}|\psi\rangle$. By use of the index notation the Schrödinger equation can be represented in the compact form $\mathrm{i}\hbar\partial_t\psi^\alpha = H^\alpha_\beta\psi^\beta$, where

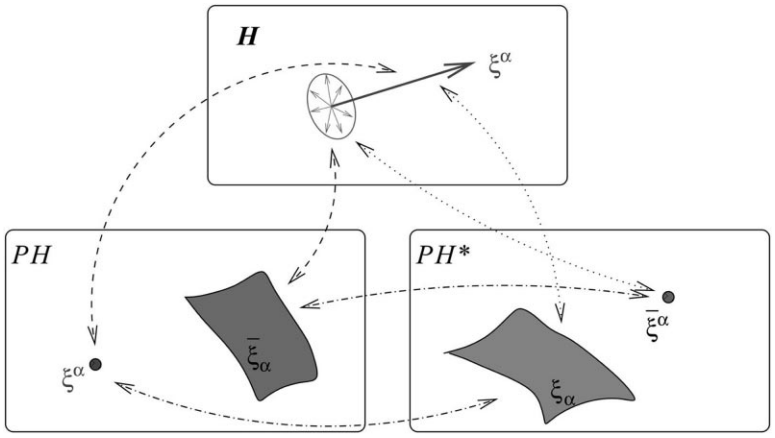

Fig. 1. *Hermitian correspondence*. A pure quantum mechanical state corresponds to a ray through the origin O in complex Hilbert space $\mathcal{H}$. Such a ray is given by a Hilbert space vector ξ^α, specified up to proportionality, which can also be used as a set of 'homogeneous coordinates' for a point in the projective Hilbert space $\mathcal{P}H$. The states ψ^α orthogonal to ξ^α constitute a projective hyperplane in $\mathcal{P}H$, with the equation $\bar{\xi}_\alpha\psi^\alpha = 0$. This hyperplane corresponds to a point $\bar{\xi}_\alpha$ in the dual projective space $\mathcal{P}H^*$.

H^α_β is the Hamiltonian operator, $\partial_t = \partial/\partial t$, and for the projective Schrödinger equation we have

$$\mathrm{i}\hbar\psi^{[\alpha}\partial_t\psi^{\beta]} = \psi^{[\alpha}H^{\beta]}_\gamma\psi^\gamma,$$

where the skew brackets indicate antisymmetrisation.

A Hilbert space vector ξ^α can also represent homogeneous coordinates for the corresponding point in the projective Hilbert space $\mathcal{P}H$. This is valid when we consider relations homogeneous in ξ^α, for which the scale is irrelevant. For example, the complex conjugate $\bar{\xi}_\alpha$ of a 'point' in $\mathcal{P}H$ can be represented by the linear subspace (hyperplane) of points ψ^α in $\mathcal{P}H$ satisfying $\bar{\xi}_\alpha\psi^\alpha = 0$. The set of all such hyperplanes constitutes the dual space $\mathcal{P}H^*$. The points of $\mathcal{P}H^*$ correspond to hyperplanes in $\mathcal{P}H$. Conversely, the points of $\mathcal{P}H$ correspond to hyperplanes in $\mathcal{P}H^*$, as indicated in Fig. 1.

One of the advantages of the use of projective geometry in the present context is that it allows us to represent states (points) and dual states (hyperplanes) as geometrical objects coexisting in the same space $\mathcal{P}H$. The complex conjugation operation, in particular, determines a *Hermitian correspondence* between points and their conjugate hyperplanes.

4. Superposition of states

The join of two distinct points ξ^α and η^α in $\mathcal{P}H$ is a complex projective line, represented by points in $\mathcal{P}H$ of the form

$$\psi^\alpha = A\xi^\alpha + B\eta^\alpha,$$

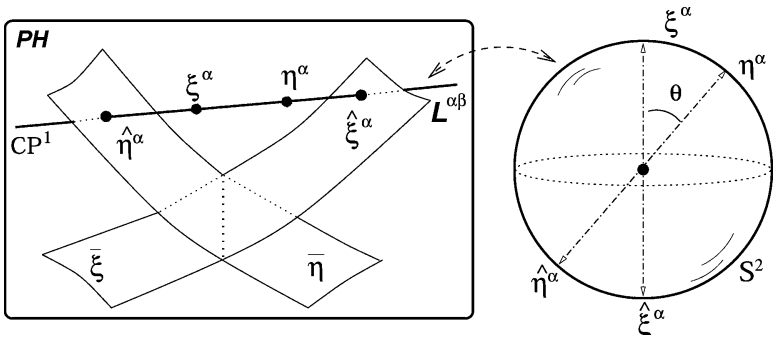

Fig. 2. *Transition probability*. The join of two states ξ^α and η^α in projective Hilbert space $\mathcal{P}H$ is a complex projective line CP^1: $L^{\alpha\beta} = \xi^{[\alpha}\eta^{\beta]}$. The points on $L^{\alpha\beta}$ represent superpositions of ξ^α and η^α. Such a line is intrinsically a real 2-manifold with spherical topology. The conjugate hyperplanes $\bar{\xi}_\alpha$ and $\bar{\eta}_\alpha$ intersect $L^{\alpha\beta}$ at points $\widehat{\xi}^\alpha$ and $\widehat{\eta}^\alpha$ in $\mathcal{P}H$. The angle θ determined by the cross-ratio $\cos^2(\theta/2) = \xi^\alpha\bar{\eta}_\alpha\eta^\beta\bar{\xi}_\beta/\xi^\gamma\bar{\xi}_\gamma\eta^\delta\bar{\eta}_\delta$ induces a metrical geometry on S^2, for which θ is the usual angular distance, and $\widehat{\xi}^\alpha$ is antipodal to ξ^α.

where A and B are complex numbers, not both zero. A neat way of characterising this line is in terms of the tensor $L^{\alpha\beta} = \xi^{[\alpha}\eta^{\beta]}$. Physically, $L^{\alpha\beta}$ represents the system of all possible quantum mechanical superpositions of the states ξ^α and η^α. Consider, e.g., the finite-dimensional case where $\mathcal{P}H = CP^n$, the n-dimensional complex projective space. Then, because of the skew-symmetry of $L^{\alpha\beta}$ it has $\frac{1}{2}n(n+1)$ complex components, which can be viewed as the line coordinates of the given line. The fundamental property of these line coordinates is that their ratios are independent of the choice of the two points ξ^α and η^α, in such a way that all points on the given line are treated on an equal footing.

The simplest situation in which a probabilistic idea arises in quantum theory is also the simplest situation in which the concept of the 'distance' between two states arises. The transition probability for the states ξ^α and η^α determines an angle θ as follows:

$$\cos^2\left(\frac{\theta}{2}\right) = \frac{\xi^\alpha\bar{\eta}_\alpha\eta^\beta\bar{\xi}_\beta}{\xi^\gamma\bar{\xi}_\gamma\eta^\delta\bar{\eta}_\delta}.$$

Clearly, θ is independent of the scale and phase of ξ^α and η^α. This angle defines a distance between the states ξ^α and η^α in $\mathcal{P}H$, as illustrated in Fig. 2. If the states coincide, then $\theta = 0$; for orthogonal states we have $\theta = \pi$, the maximum distance.

Suppose we set $\theta = \mathrm{d}s$ and $\xi^\alpha = \psi^\alpha$, $\eta^\alpha = \psi^\alpha + \mathrm{d}\psi^\alpha$. By use of the expression for the transition probability, expanded to second order, we find that the infinitesimal distance $\mathrm{d}s$ between two neighbouring states is

$$\mathrm{d}s^2 = 8\left[\frac{\psi^{[\alpha}\,\mathrm{d}\psi^{\beta]}\bar{\psi}_{[\alpha}\,\mathrm{d}\bar{\psi}_{\beta]}}{(\bar{\psi}_\gamma\psi^\gamma)^2}\right],$$

an expression known to geometers as the Fubini–Study metric [9,58]. This metric is well defined both in finite and infinite dimensions (see, e.g., [60]). The introduction of the Fubini–Study metric illustrates how the notions of probability and distance become interlinked, once quantum theory is formulated in a geometric manner. The *geodesic distance*

with respect to the Fubini–Study metric determines the transition probability between two states. Indeed, the nontrivial metrical geometry of the Fubini–Study manifold is responsible for the 'peculiarities' of the quantum world, and in what follows we shall see various examples of this phenomenon.

5. Spin measurements

The specification of a physical system implies further geometrical structure on the state space. The point of view we suggest is that *all* the relevant physical details of a quantum system can be represented by additional projective geometrical features. Here and in subsequent sections we shall illustrate this point with several examples. Let us first consider the spin degrees of freedom of a nonrelativistic spin 1 particle, as represented by a symmetric spinor ϕ^{AB} ($A, B = 0, 1$). The relevant Hilbert space has three dimensions, and we denote the corresponding projective Hilbert space CP^2. A symmetric spinor has a natural decomposition $\phi^{AB} = \alpha^{(A}\beta^{B)}$, where α^A and β^A are called 'principal spinors', and round brackets denote symmetrisation. There is a special conic $\mathcal{C}$, corresponding to degenerate spinors of the form $\phi^{AB} = \psi^A\psi^B$ for some repeated principal spinor ψ^A.

The identification of $\mathcal{C}$ is sufficient to induce the structure of a spin 1 system on the state space, since through any generic point in CP^2 there are two lines tangent to $\mathcal{C}$, and the corresponding tangent points determine the principal spinors, up to scale, as shown in Fig. 3. Alternatively, we can think of a conic $\mathcal{C}$ in CP^2 being represented by a map (see, e.g., [83]) from CP^1 to CP^2 such that if (t, u) are homogeneous coordinates on CP^1, we have the Veronese embedding

$$\mathcal{C} : (t, u) \to (t^2, tu, u^2),$$

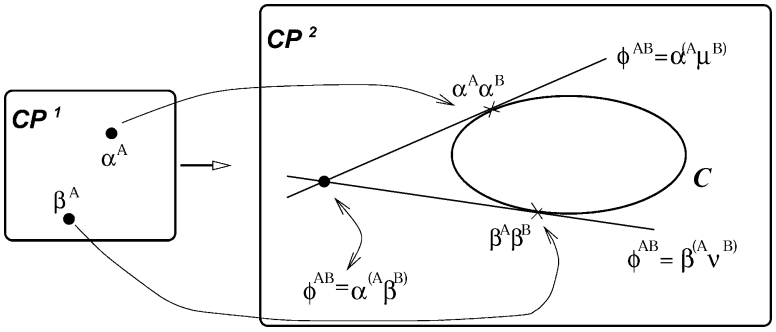

Fig. 3. *Spin* 1 *particle*. A symmetric spinor ϕ^{AB} has three independent components which act as homogeneous coordinates for CP^2. The image of the map $\mathcal{C} : CP^1 \to CP^2$, defined by $\{\psi^A \in CP^1\} \to \{\psi^A\psi^B \in CP^2\}$ determines a curve $\mathcal{C}$ in CP^2. The tangent to $\mathcal{C}$ at the point $\phi^{AB} = \alpha^A\alpha^B$ in CP^2 consists of spinors of the form $\phi^{AB} = \alpha^{(A}\mu^{B)}$ for some μ^A. The intersection of the lines tangent to the points $\alpha^A\alpha^B$ and $\beta^A\beta^B$ is the point $\alpha^{(A}\beta^{B)}$. Conversely, once a conic $\mathcal{C}$ is specified, a map $\mathcal{C}^{-1}$ is established from CP^2 to point-pairs in CP^1, called principal spinors. The points on $\mathcal{C}$ map to degenerate point-pairs.

where (t^2, tu, u^2) now represent homogeneous coordinates on CP^2. Because a complex projective line, in real terms, represents a sphere S^2 (see Fig. 2), the specification of the spin direction in $\mathbb{R}^3$ determines a point on S^2, and hence on $\mathcal{C}$.

For quantum mechanics the conic is required to be compatible with the complex conjugation operation on the state space in the sense that if we conjugate a point of $\mathcal{C}$, then the resulting line is tangent to $\mathcal{C}$. If in algebraic terms the conic is given by $C_{\alpha\beta}\xi^\alpha\xi^\beta = 0$, then we require $C^{\alpha\beta} = \bar{C}^{\alpha\beta}$, where $C^{\alpha\beta}$ and $\bar{C}^{\alpha\beta}$ are, respectively, the inverse and the complex conjugate of $C_{\alpha\beta}$. The complex conjugate $\bar{\phi}_{AB} = \bar{\alpha}_{(A}\bar{\beta}_{B)}$ of a general state corresponds to a complex projective line consisting of states of the form $P\bar{\alpha}^A\bar{\alpha}^B + Q\bar{\beta}^A\bar{\beta}^B$ for arbitrary complex P and Q (not both vanishing). Here we define $\bar{\alpha}^A = \epsilon^{AB}\bar{\alpha}_B$ and $\bar{\beta}^A = \epsilon^{AB}\bar{\beta}_B$, with ϵ^{AB} the natural symplectic structure. The rules for the complex conjugation map $\mathbf{c}$ on spinors are given, more explicitly, by $\mathbf{c}(\alpha^A) = \bar{\alpha}_A$ and $\mathbf{c}(\bar{\alpha}^A) = -\alpha_A$. The latter identity arises since $\mathbf{c}(\bar{\alpha}^A) = \mathbf{c}(\epsilon^{AB}\bar{\alpha}_B) = \epsilon_{AB}\alpha^B = -\alpha_A$.

Recall in this connection that for any spinor ϕ^A we have the relations $\phi^A = \epsilon^{AB}\phi_B$ and $\phi^A\epsilon_{AB} = \phi_B$, and that ϵ_{AB} satisfies $\epsilon_{AB} = -\epsilon_{BA}$ and $\epsilon_{AB} = \bar{\epsilon}_{AB}$. If we take the complex conjugate of a state on $\mathcal{C}$, the resulting line is tangent to the conic at a point, which we call the conjugate of the original point on $\mathcal{C}$. This establishes a Hermitian correspondence between pairs of points on $\mathcal{C}$. For a state $\phi^{AB} = \psi^A\psi^B$ the conjugate line consists of states of the form $\lambda^{(A}\bar{\psi}^{B)}$ for arbitrary λ^A. This line touches the conic $\mathcal{C}$ at the point $\bar{\psi}^A\bar{\psi}^B$.

Each choice of a point on $\mathcal{C}$, as noted above, determines a spin axis. For any spin axis there are three possible spin states, with eigenvalues 1, −1 and 0. The spin eigenstates are the points $\psi^A\psi^B$ and $\bar{\psi}^A\bar{\psi}^B$ on $\mathcal{C}$, having the eigenvalues 1 and −1, together with a third point $\psi^{(A}\bar{\psi}^{B)}$ obtained by intersecting the lines tangent to the conic $\mathcal{C}$ at the other two points, corresponding to eigenvalue 0, as indicated in Fig. 4.

When a spin measurement is made, the initial state corresponds to a generic point X in CP^2, and the measurement is defined by a spin axis. The state then 'jumps' from its initial point to one of the three spin eigenstates associated with the choice of axis. Quantum theory, as such, states nothing about the 'mechanism' whereby this jump is achieved.

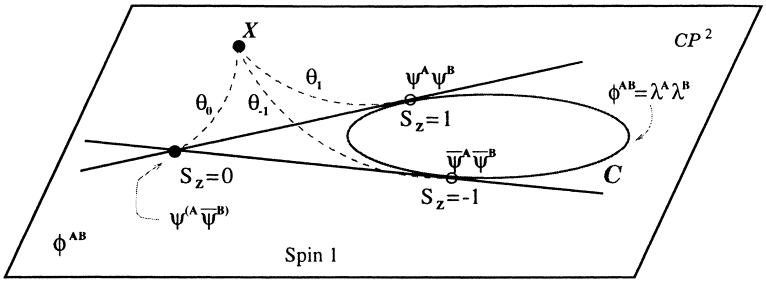

Fig. 4. *Spin measurement*. The state space of a spin 1 system has a conjugation relation that associates to each point $\psi^A\psi^B$ on the special conic a conjugate point $\bar{\psi}^A\bar{\psi}^B$. The antipodal points ψ^A and $\bar{\psi}^A$ on the corresponding 2-sphere select a direction in Euclidean 3-space. The three points $\psi^A\psi^B$, $\bar{\psi}^A\bar{\psi}^B$ and $\psi^{(A}\bar{\psi}^{B)}$ are eigenstates of the spin operator S_z associated with this axis. The corresponding geodesic distances $\theta_1, \theta_{-1}, \theta_0$ to a generic state $X \in CP^2$ determine the probabilities of the measurement outcomes for S_z for a particle in the initial state X.

We can, however, compute the probabilities, and describe the result in geometrical terms. First we calculate the distance from X to each of the three spin eigenstates, by use of the Fubini–Study metric. This gives us three angles θ_1, θ_{-1}, and θ_0. For each angle we compute $P(\theta) = \frac{1}{2}(1 + \cos\theta)$, which gives us the probability of transition to that particular state. It is not obvious that the three probabilities computed in this way sum up to 1, given any initial state in which the measurement is performed, but they do: this is a 'miracle' of the Fubini–Study geometry.

6. Spin $\frac{3}{2}$ and the twisted cubic curve

We have seen that in the case of a projective plane, there is a conic $\mathcal{C}$, corresponding to degenerate spinors obtained by a special map from a projective line to a plane. On the other hand, in three-dimensional projective space CP^3 there are two different kinds of locus to be considered, each of which is in some respects a proper analogue of the conic, namely, the quadric surface Q and the twisted cubic curve $\mathcal{T}$. While a surface is the locus of a variable point of space which has two complex degrees of freedom, a curve is the locus of a variable point of space of one complex degree of freedom. When viewed as the state space of a quantum mechanical system, the quadric surface in CP^3 characterises the disentangled states of a pair of spin $\frac{1}{2}$ particles, the geometry of which we shall study in some detail in Sections 8–10.

The twisted cubic, the simplest nonplanar curve in projective geometry, on the other hand, plays an essential role in the geometry of the state space of a spin $\frac{3}{2}$ particle. Analogous to the conic curve, the twisted cubic can be represented by a map from CP^1 to CP^3 of the form

$$\mathcal{T} : (t, u) \to (t^3, t^2u, tu^2, u^3),$$

where (t^3, t^2u, tu^2, u^3) represents the homogeneous coordinates of a point on $\mathcal{T}$ in CP^3. It follows that $\mathcal{T}$ is an algebraic space of the third degree, which meets a generic plane of CP^3 in three points.

In order to proceed further, we introduce a spinorial notation and let the symmetric spinor $\psi^{ABC} = \psi^{(ABC)}$ denote homogeneous coordinates on CP^3 [54]. Then, the twisted cubic curve is determined by the relation $\tau_{AB} = 0$, where

$$\tau_{AB} \triangleq \psi_{CD(A}\psi_{B)}{}^{CD}.$$

As a consequence we see that $\mathcal{T}$ is given by the common intersection of two-dimensional net of quadric surfaces in CP^3. Here the indices on ψ^{ABC} are raised and lowered according to the standard conventions, so, e.g., $\psi_B^{CD} = \epsilon_{AB}\psi^{ACD}$. The general solution to the algebraic relations given by $\tau_{AB} = 0$ takes the form $\psi^{ABC} = \xi^A\xi^B\xi^C$ for arbitrary ξ^A. Then if we parametrise a point $\xi^A \in CP^1$ according to the scheme $\xi^A = (t, u)$, we recover the map $\tau : CP^1 \to CP^3$ noted above.

The specification of a twisted cubic $\mathcal{T}$ in CP^3 induces a *null polarity* on the state space, i.e., a natural correspondence between points and planes such that the polar plane of a given point includes that point. The null polarity is given by the map

$$\psi^{ABC} \to \psi_{ABC} = \epsilon_{AP}\epsilon_{BQ}\epsilon_{CR}\psi^{PQR}$$

and it follows as an elementary spinor identity that $\psi^{ABC}\psi_{ABC} = 0$ for any choice of ψ^{ABC}. In the case of a point $\psi^{ABC} = \xi^A\xi^B\xi^C$ on $\mathcal{T}$, the corresponding polar plane intersects $\mathcal{T}$ solely at that point, with a threefold degeneracy, and is called the *osculating plane* at that point.

Through a given point $\xi^A\xi^B\xi^C \in \mathcal{T}$, the associated tangent line is given by points of the form $\xi^{(A}\xi^B\eta^{C)}$, with η^A arbitrary. We say that a generic point of CP^3, with three distinct principal spinors, is of type {1, 1, 1}. The point that lie on tangents to $\mathcal{T}$ are of type {2, 1}, whereas the points of $\mathcal{T}$ are of type {3}. A necessary and sufficient condition for a point to be of type {2, 1} is the vanishing of the invariant $\mathcal{G} = \tau_{AB}\tau^{AB}$. Hence we see that the tangent lines to $\mathcal{T}$ generates a quartic surface $\mathfrak{G}$ in CP^3.

For quantum mechanics the twisted cubic has to be self-conjugate in the sense that the complex conjugate plane of any point on $\mathcal{T}$ has to be the osculating plane of another point on $\mathcal{T}$. The choice of a point on $\mathcal{T}$ determines a spin axis. For each spin axis, there are four possible spin eigenstates, with eigenvalues $\frac{3}{2}$, $\frac{1}{2}$, $-\frac{1}{2}$ and $-\frac{3}{2}$. Two of the spin states, corresponding to the eigenvalues $\pm\frac{3}{2}$, lie on $\mathcal{T}$ itself. These two states can be written $\psi^A\psi^B\psi^C$ and $\bar{\psi}^A\bar{\psi}^B\bar{\psi}^C$, where $\bar{\psi}^A = \epsilon^{AB}\bar{\psi}_B$ and $\bar{\psi}_B = \mathbf{c}(\psi^B)$.

The complex conjugate of the state $\psi^{ABC} = \psi^A\psi^B\psi^C$ on the twisted cubic $\mathcal{T}$ is the plane $\bar{\psi}_{ABC} = \bar{\psi}_A\bar{\psi}_B\bar{\psi}_C$ in CP^3, and this plane osculates $\mathcal{T}$ at the point $\bar{\psi}^A\bar{\psi}^B\bar{\psi}^C$. Through the point $\psi^A\psi^B\psi^C$ there is a unique line tangent to $\mathcal{T}$, and this line intersects the plane $\bar{\psi}_A\bar{\psi}_B\bar{\psi}_C$ at the point $\psi^{(A}\psi^B\bar{\psi}^{C)}$. This point is the spin $\frac{1}{2}$ eigenstate with respect to that choice of axis. Conversely, the tangent line to $\mathcal{T}$ at the spin $-\frac{3}{2}$ state $\bar{\psi}^A\bar{\psi}^B\bar{\psi}^C$ intersects the osculating plane of $\mathcal{T}$ at $\psi^A\psi^B\psi^C$ at the point $\bar{\psi}^{(A}\bar{\psi}^B\psi^{C)}$, which is the spin $-\frac{1}{2}$ state, as illustrated in Fig. 5. That concludes our identification of the four possible spin eigenstates that can arise with respect to a given choice of axis.

An interesting feature of the twisted cubic geometry arises from the fact that for any symmetric spinor ψ^{ABC} we have the syzygistic relation

$$\tau_{AB}\psi^{ABC} = 0,$$

which follows from the spinor identity $\epsilon_{[AB}\epsilon_{C]D} = 0$. This formula implies that through any point ψ^{ABC} in $CP^3 - \mathfrak{G}$, i.e., a point off the quartic surface, there exists a unique chord of $\mathcal{T}$. This follows from the fact that, providing τ_{AB} is nondegenerate, the condition $\tau_{AB}\psi^{ABC} = 0$ implies a relation of the form

$$\psi^{ABC} = u\xi^A\xi^B\xi^C + v\eta^A\eta^B\eta^C$$

for some ξ^A and η^A corresponding to a pair of spin axes such that $\xi_A\eta^A \neq 0$, where (u, v) are homogeneous coordinates on CP^1. It follows that an arbitrary quantum state ψ^{ABC} in $CP^3 - \mathfrak{G}$ admits a unique characterisation as a superposition of a pair of spin $\frac{3}{2}$ eigenstates

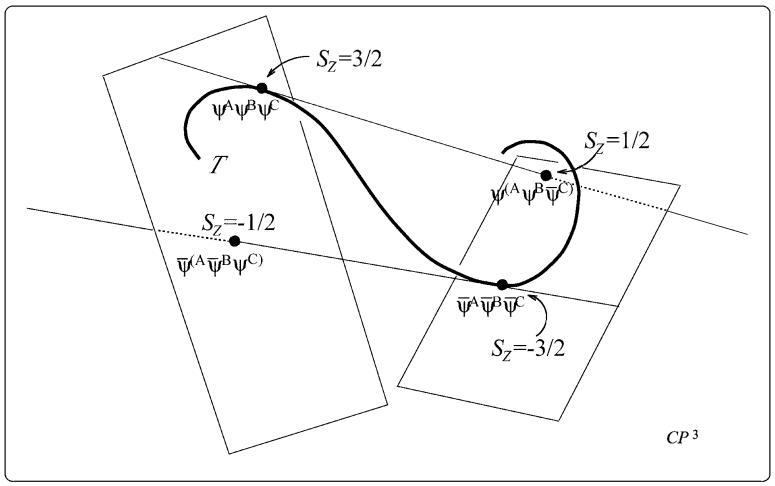

Fig. 5. *The twisted cubic curve as a system of spin states*. The quantum phase space for a spin $\frac{3}{2}$ particle contains a preferentially identified twisted cubic $\mathcal{T}$ which is self-conjugate in the sense that the complex conjugate plane corresponding to any point on $\mathcal{T}$ necessarily osculates the curve at some other point on $\mathcal{T}$, which we regard as conjugate to the original point. The points of $\mathcal{T}$ are those states which have an eigenstate of spin $\frac{3}{2}$ relative to some choice of spin axis. Each point of $\mathcal{T}$ corresponds to a choice of spin axis and direction, and its conjugate corresponds to the same axis with a reverse of direction.

corresponding to distinct spin axes. If τ_{AB} is degenerate, then the chord reduces to a tangent line to $\mathcal{T}$ with a double point at the intersection, and ψ^{ABC} has a unique representation of the form $\psi^{ABC} = \xi^{(A}\xi^B\eta^{C)}$.

7. The rational quartic curve and spin 2 systems

A similar analysis to that described in this section can also be pursued in connection with the geometry of a spin 2 system, for which the state space is CP^4, endowed with a self-conjugate rational quartic curve. The geometry of this curve is closely related to the Petrov classification of gravitational fields as developed in its modern form by Penrose [68] and others. See, e.g., [71,72,76] for references and further relevant details.

In this connection we note that there are two levels of specialisation in the description of the state space. If we take CP^4 with the Fubini–Study metric, but without the specification of a self-conjugate rational quartic curve, then we have the state space appropriate for a generic five-state system. If we take CP^4 with the rational quartic without the Fubini–Study geometry, then we have the set-up appropriate for the geometry of gravitational fields, but without bringing quantum mechanics into play. That is the situation where the Petrov scheme arises. Finally, when we bring both the rational quartic and the Fubini–Study metric into the picture, we have the state space geometry for a spin 2 quantum system.

Let us consider first the case when we have a rational quartic curve R in CP^4, but without consideration of the metric. For a general treatment of the properties of this curve, see, e.g.,

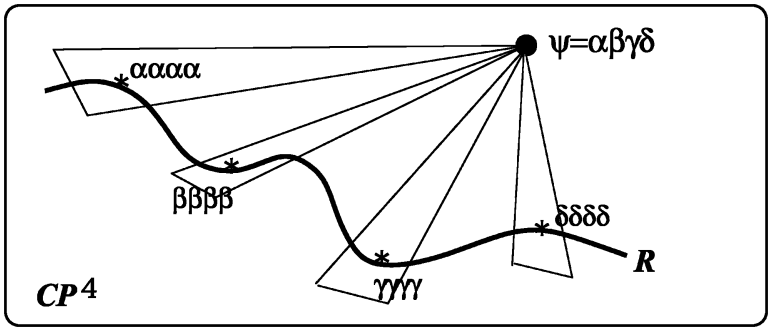

Fig. 6. *The Petrov classification*. Passing through a generic point $\psi^{ABCD} = \alpha^{(A}\beta^{B}\gamma^{C}\delta^{D)}$ in CP^4 there are four osculating solids of the rational quartic curve $\mathcal{R}$. The points on $\mathcal{R}$ where these solids touch determine the four principal spinors. A degeneracy of type $\{2, 1, 1\}$ occurs if two of the solids coincide, and ψ^{ABCD} lies on an osculating 2-plane. When three solids coincide, we find that ψ^{ABCD} is of type $\{3, 1\}$ and lies on a tangent line. When all four solids coincide, ψ^{ABCD} is of type $\{4\}$ and lies on $\mathcal{R}$. The type $\{2, 2\}$ case arises when ψ^{ABCD} is an intersection point of a pair of osculating 2-planes.

[88]. The rational quartic is given by the Veronese embedding $\mathcal{R} : CP^1 \to CP^4$, given by

$$\mathcal{R} : (t, u) \to (t^4, t^3u, t^2u^2, tu^3, u^4).$$

In spinor terms, a point on $\mathcal{R}$ is necessarily of the form

$$\psi^{ABCD} = \alpha^A\alpha^B\alpha^C\alpha^D$$

for some choice of $\alpha^A \in CP^1$. The points on $\mathcal{R}$ thus correspond to 'null' gravitational spinors, i.e., spinors of Petrov type $\{4\}$, with a fourfold degeneracy in the principal spinors.

Associated with any point of $\mathcal{R}$ are three special linear spaces. These are the tangent line, the osculating plane, and the osculating solid. The tangent line at the fixed point $\alpha^A\alpha^B\alpha^C\alpha^D \in \mathcal{R}$ consists of spinors of the form $\alpha^{(A}\alpha^B\alpha^C\beta^{D)}$ for some choice of β^A. The osculating plane consists of spinors of the form $\alpha^{(A}\alpha^B\beta^C\gamma^{D)}$ and for the osculating solid we have spinors of the form $\alpha^{(A}\beta^B\gamma^C\delta^{D)}$. Four osculating solids, corresponding to the four principal spinors, pass through a generic point of CP^4, as illustrated in Fig. 6.

The various types of degeneracies that can arise can be given an elegant characterisation in terms of the geometry of the rational quartic curve. Here we follow a procedure very similar to the cases described for spin 1 and spin $\frac{3}{2}$ (cf. [54,67]). The spinors of type $\{3, 1\}$ or type $\{4\}$ constitute together a sextic 2-surface $\mathfrak{M} \in CP^4$ ruled by the tangent lines of $\mathcal{R}$. A necessary and sufficient condition for a spinor to lie on $\mathfrak{M}$ is the vanishing of the invariants

$$\mathcal{I} = \psi_{ABCD}\psi^{ABCD}, \qquad \mathcal{J} = \psi_{AB}{}^{CD}\psi_{CD}{}^{EF}\psi_{EF}{}^{AB}.$$

The spinors of type $\{2, 1, 1\}$, $\{3, 1\}$, $\{2, 2\}$ and $\{4\}$ constitute together a sextic primal $\mathfrak{D}$ in CP^4 given by the equation $\mathcal{I}^3 = 6\mathcal{J}^2$. This is a necessary and sufficient condition for ψ^{ABCD} to lie on an osculating plane of $\mathcal{R}$. More generally, we note that $CP^4 - \mathfrak{M}$ is foliated by a pencil of sextic primals with base $\mathfrak{M}$, given by $p\mathcal{I}^3 = q\mathcal{J}^2$, where p, q (not both

vanishing) are homogeneous coordinates for a point in CP^1. The spinors of type $\{2,2\}$ or $\{4\}$ lie together on a two-dimensional quartic subsurface $\mathfrak{K}$ of the sextic primal $\mathfrak{D}$, given by the equation

$$\psi_{(ABC}{}^{K}\psi_{DE}{}^{LM}\psi_{F)KLM}=0,$$

which can be interpreted as the common intersection locus of a six-dimensional net of cubic primals. The surface $\mathfrak{K}$ is generated by intersections of pairs of osculating 2-planes.

When quantum theory is brought into the picture, we augment the operations indicated above with the requirement that the rational quartic curve should be self-conjugate in the sense that the complex conjugate of the polar solid of a point on $\mathcal{R}$ is another point on $\mathcal{R}$. The polar solid of a general point in CP^4 with respect to $\mathcal{R}$ is defined to be the solid spanned by the tangential points of the four osculating planes through the given point.

For a point on $\mathcal{R}$, the polar solid is defined to be the osculating plane at that point. The complex conjugate of this polar solid is a point which we call the complex conjugate of the original point. We require that if the original point is on $\mathcal{R}$, then so is its complex conjugate. The choice of a point on $\mathcal{R}$ determines a spin-axis, and the complex conjugate of this point then corresponds to the same axis but with the orientation reversed. In particular, the chosen state on $\mathcal{R}$ has $S_z=2$ with respect to the corresponding z-axis, and the complex conjugate states has $S_z=-2$. The $S_z=1$ state obtained by intersecting the tangent line of an $S_z=2$ state with the osculating solid of the corresponding $S_z=-2$ state. The $S_z=-1$ state is obtained by intersecting the osculating solid of the $S_z=2$ state with the tangent line of the $S_z=-2$ state. Finally, the $S_z=0$ state is the point obtained by intersecting the osculating planes at $S_z=2$ and $S_z=-2$ states, as illustrated in Fig. 7. We remark, incidentally, that the $S_z=0$ states are 'real' in the sense that $\psi^{ABCD}\propto\bar{\psi}^{ABCD}$ for these points. Thus the $S_z=0$ states are given by the real points of the surface $\mathfrak{K}$.

In contrast with the spin $\frac{3}{2}$ case, where a general state can be expressed in a unique way as a superposition of a pair of $S_z=\frac{3}{2}$ states for two choices of spin axis, it is generally not true that a spin 2 state can be expressed as a superposition of a pair of $S_z=2$ states. For this we require that ψ^{ABCD} should lie on a chord of $\mathcal{R}$, a necessary and sufficient condition for which is given by the vanishing of the cubic invariant $\mathcal{J}$. An equivalent way of stating that ψ^{ABCD} should lie on the chordal primal $\mathcal{J}=0$ is that the four principal spinors should satisfy the harmonic condition. On the other hand, passing through a general state ψ^{ABCD} there exists a one-parameter family of trisecant planes, each of which cuts the twisted quartic at three points, thus allowing us to express ψ^{ABCD} as a sum of three $S_z=2$ states in ∞^1 ways. The locus generated by the trisecant planes through a general state is a quadric cone.

8. Geometry of entanglement

Now we consider the spin degrees of freedom of an entangled pair of spin $\frac{1}{2}$ particles. The generic two-particle state ψ^{AB} for a pair of such particles (e.g., an electron and a positron) has a four-dimensional Hilbert space, and the state space is CP^3. There is a preferred point Z in CP^3, corresponding to the singlet state of total spin 0, for which $\psi^{AB}=\psi^{[AB]}$. The

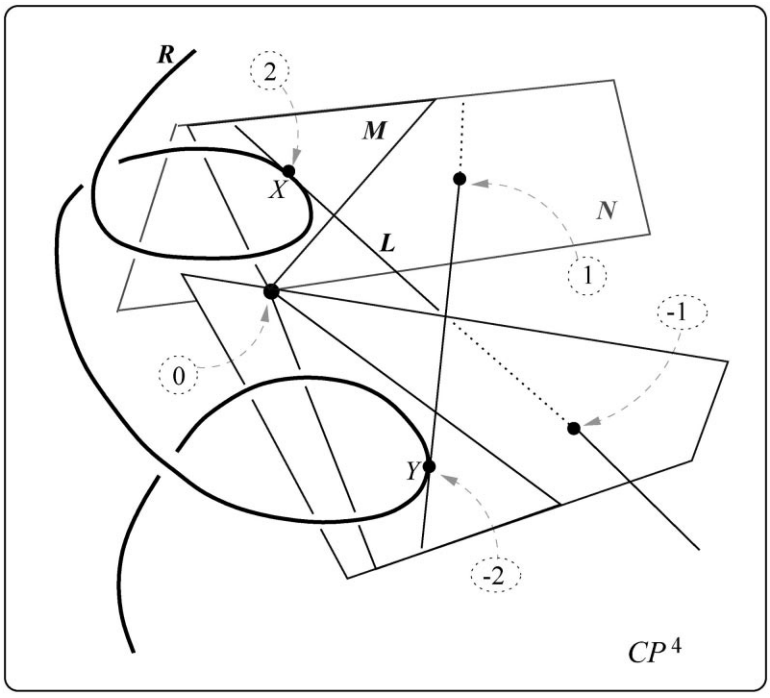

Fig. 7. *Geometry of the rational quartic curve*. At a generic point A on the curve $\mathcal{R}$ we can draw the tangent line L, which lies in the osculating 2-plane M at A, which lies in the osculating 3-solid N at A. If B is another point on $\mathcal{R}$, then the tangent line O to R at B lies in the osculating 2-plane P at B, which lies in the osculating 3-solid Q at B. The tangent to $\mathcal{R}$ at A meets the osculating solid Q at C. The tangent to $\mathcal{R}$ at B meets the osculating solid N at D. The osculating plane M at A intersects the osculating plane P at B at the point E. For a spin 2 system, the curve $\mathcal{R}$ is self-conjugate: the complex conjugate hyperplane to a point on $\mathcal{R}$ is the osculating solid of another point on $\mathcal{R}$. The choice of a point on $\mathcal{R}$ determines a spin axis. If A and B are conjugate, the eigenstates of the spin operator S_z with eigenvalues 2, 1, 0, -1, -2 are given by the points A, C, E, D, B, respectively.

conjugate plane $\bar{Z}$ contains the triplet states of total spin 1, for which $\psi^{AB} = \psi^{(AB)}$. We note that $\bar{Z}$ is endowed with a self-conjugate conic $\mathcal{C}$, each point of which defines a spin axis. There is also a surface $Q \in CP^3$, given by the quadratic equation

$$\epsilon_{AC}\epsilon_{BD}\psi^{AB}\psi^{CD} = 0,$$

consisting of states of the *disentangled* form $\psi^{AB} = \xi^A\eta^B$, representing an embedding of the product of the state spaces of the individual spin $\frac{1}{2}$ particles. The pure states off the quadric are the *entangled* states.

Suppose we start with a combined state of total spin 0 for the two particles, and we measure the spin of the first particle (say, the electron) relative to a given choice of axis. This will disentangle the state, so the result lies on Q. The choice of axis and orientation determines a point and its conjugate on the conic $\mathcal{C}$. The tangents to the conic at these points intersect to form a third point off the quadric but in the plane of total spin 1, corresponding

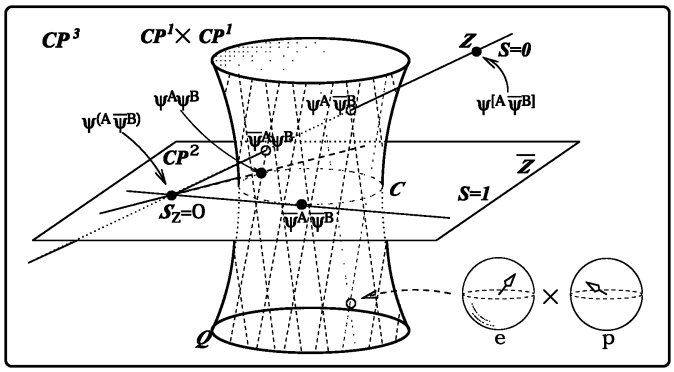

Fig. 8. *Quantum entanglement*. The quantum phase space of an electron–positron system contains a point Z for total spin 0, and a projective hyperplane $\bar{Z}$ for total spin 1. The disentangled states have indefinite total spin, and comprise a quadric $Q \in CP^3$ ruled by two systems (electron and positron) of linear generators. Once a spin axis is chosen, the join of Z with the state of total spin 1 and $S_z = 0$ intersects Q in a pair of points, corresponding to the possible measurement outcomes of the spin of the electron relative to the axis.

to a triplet state of eigenvalue 0 relative to the axis. We join that state to the starting state Z, and the resulting line intersects Q at a pair of points, as shown in Fig. 8.

The two disentangled states thus obtained represent the possible measurement outcomes. The quadric Q has two systems of generators, corresponding to the electron and positron state spaces. Through each point of Q there is a unique 'electron generator' and a unique 'positron generator'. An electron generator represents a fixed electron state, each point on it corresponding to a possible positron state. The two points constituting the possible outcomes of the spin measurement of the electron have the property that their electron generators hit respectively the two chosen points on the conic that define the spin axis. The measurement result for which the electron generator hits the spin up state on the conic is the 'electron spin up and positron spin down' outcome, whereas the other one is the 'electron spin down and positron spin up' outcome. The argument outlined above are clearly relevant to the formulation of a proper geometric treatment of the EPR problem, though in that situation one must also take into account the further degrees of freedom associated with the geometry of space–time.

In the case of a measurement upon a generic state, not necessarily of total spin 0, the possible resulting outcomes are constructed geometrically as follows. Without loss of generality, we consider, in the present set-up, the measurement of the spin of the electron with respect to a spin axis. The choice of the spin axis selects a pair of points on the conic in Q. Each of these points determines a corresponding electron generator. The two electron generators thus obtained do not meet. Now given a generic point and a pair of skew lines in CP^3, there exists a unique line through this point that intersects the two lines transversally. The line thus obtained necessarily intersects Q at two points, and these two points determine the two possible measurement outcomes of the electron spin with respect to that choice of axis.

In a more general situation, the idea of the quantum entanglement of a system of particles is characterised geometrically by the fact that complex projective space admits a Segre

embedding (cf. [42]) of the form

$$CP^m \times CP^n \hookrightarrow CP^{(m+1)(n+1)-1}.$$

Here we regard both CP^m and CP^n as representing the state space of two subsystems, respectively, while $CP^{(m+1)(n+1)-1}$ represents the state space of the combined system. One can argue that this is the main feature of quantum mechanics that has no analogue is classical physics. Classically, the state space of a combined system is given by the product of the state spaces of the subsystems, which typically has much lower dimensionality than the quantum state space of a combined system.

One should bear in mind that there are two distinct categories of order and disorder that can enter into the characterisation of a multi-particle quantum system. One has to do with thermalisation: the admixture of pure quantum states into a Gibbsian ensemble. The other category of order–disorder relation is concerned with degree of entanglement. The laws of thermodynamics must account for a general tendency towards both mixing as well as disentanglement. The latter is in some respects more elusive, and it is not clear a priori how to formulate a physical basis for the process of disentanglement, which does not admit a simple description in the language of thermodynamics. One of the motivations behind the present study is to establish a satisfactory framework for exploring this issue further.

9. Measure of entanglement

The geometrical set-up indicated in the previous section suggests a methodology according to which a measure $\Delta(\psi)$ can be assigned to the *degree of entanglement* exhibited by a given pure state ψ. Let us consider, e.g., the case of a finite-dimensional two-particle state space CP^n containing a variety $V^m \subset CP^n$, where $V^m = CP^j \times CP^k$ and $n = (j+1)(k+1)-1$. The variety V^m represents the disentangled states of the two particles, and is given by the product of the respective single particle state spaces CP^j and CP^k.

We propose, as a measure of entanglement for a generic pure state $\psi \in CP^n$, the use of the *geodesic distance from the given state ψ to the nearest disentangled state*. The distance Δ is measured with respect to the Fubini–Study metric.

The choice of Δ is *natural* inasmuch as it depends only on the Segre embedding of the variety V^m and no additional structure apart from the given metrical geometry of CP^n. Furthermore, Δ is invariant under any unitary transformation of CP^n that is also an automorphism of V^m, i.e., 'local' transformations that preserve the disentangled state space. This invariance is a key property for a measure of entanglement [14,59,79,85]. Essentially the same construction applies to the case of entangled states of any number of particles. We do not require that the particles are necessarily of the same type.

As an illustration, we consider in more detail the system described in Section 8 consisting of two spin $\frac{1}{2}$ particles, where the state space is CP^3 and the space V^2 of disentangled states is a quadric $Q \subset CP^3$. Suppose we write ψ^{AB} for a generic state, and $\bar{\psi}_{AB}$ for the

corresponding complex conjugate hyperplane. Then the minimal distance Δ from ψ to Q is determined by the relation $\kappa = \frac{1}{2}(1 + \cos\Delta)$, where κ is the cross-ratio

$$\kappa = \frac{(\psi^{AB}\bar{X}_{AB})(X^{CD}\bar{\psi}_{CD})}{(\psi^{AB}\bar{\psi}_{AB})(X^{CD}\bar{X}_{CD})}$$

and $X^{AB} \in Q$ maximises κ for the given state ψ^{AB}. The cross-ratio κ is the Dirac transition probability from the state ψ^{AB} to the state X^{AB}. Our goal is to find the states on Q for which the transition probability from ψ^{AB} is maximal, corresponding to a minimal Fubini–Study distance.

We shall turn to the details of the maximisation problem in Section 10, but first we present the solution and analyse its consequences. Let us write $\psi_{CD} \triangleq \epsilon_{AC}\epsilon_{BD}\psi^{AB}$ and $\bar{\psi}^{AB} \triangleq \epsilon^{AC}\epsilon^{BD}\bar{\psi}_{AB}$, where the antisymmetric spinor ϵ_{AB} satisfies $\epsilon_{AB}\epsilon^{AC} = \delta^C_B$. Then the solution for κ is $\kappa = \frac{1}{2}(1 + \gamma)$, with

$$\gamma = \sqrt{1 - \frac{(\psi^{AB}\psi_{AB})(\bar{\psi}^{CD}\bar{\psi}_{CD})}{(\psi^{AB}\bar{\psi}_{AB})^2}}.$$

We note that γ as thus defined is independent of the scale of ϵ_{AB} and lies in the range $0 \leq \gamma \leq 1$. The inequality satisfied by γ follows from a general result that for any element $\mathbf{z}$ in a complex vector space with a Hermitian inner product we have the Hermitian inequality $(\mathbf{z}\cdot\bar{\mathbf{z}})^2 \geq (\mathbf{z}\cdot\mathbf{z})(\bar{\mathbf{z}}\cdot\bar{\mathbf{z}})$. This can be seen by writing $\mathbf{z} = \mathbf{a} + \mathrm{i}\mathbf{b}$, where $\mathbf{a}$ and $\mathbf{b}$ are real, and then checking that the purported relation reduces to the Schwartz inequality $(\mathbf{a}\cdot\mathbf{b})^2 \leq (\mathbf{a}\cdot\mathbf{a})(\mathbf{b}\cdot\mathbf{b})$. Furthermore, we can verify that γ is invariant under local transformations, i.e., unitarity transformations of the form $\psi^{AB} \to U^A_C U^B_D \psi^{CD}$, where U^A_B is an element of $U(2)$. This follows as a consequence of the fact that $\psi^{AB}\psi_{AB} \to \det(U)\psi^{AB}\psi_{AB}$ under a local transformation where $\det(U) = \epsilon_{AB}U^A_C U^B_D \epsilon^{CD}$ is evidently a pure phase.

If the point ψ^{AB} lies on the quadric Q, we have $\psi_{AB}\psi^{AB} = 0$, and hence $\gamma = 1$, which implies $\kappa = 1$, from which it follows that the distance to the quadric is $\Delta = 0$. On the other hand, for a maximally entangled state the inequality is saturated at $\gamma = 0$, and thus gives $\kappa = \frac{1}{2}$, which implies $\Delta = \pi/2$.

The interpretation of this result is as follows. We recall that for orthogonal states the Fubini–Study distance is π, the greatest distance possible. On the other hand, the maximum distance an entangled state can have from the closest disentangled state, in the case of two spin $\frac{1}{2}$ particles, is $\pi/2$. For example, with respect to a given choice of spin axis, the spin 0 singlet state ϵ^{AB} can be expressed as an antisymmetric superposition of two disentangled states, i.e., an up-down state and a down-up state. The two disentangled states are mutually orthogonal, and the singlet state lies 'half way' between them.

10. Maximal and sub-maximal entanglement

There is a well-known construction in algebraic geometry according to which a proper quadric locus in CP^3 induces a *polarity* on this space, a one-to-one correspondence between

points and planes. Reverting briefly to the notation of Section 3, let us write ψ^α for the homogeneous coordinates of a point in CP^3, and $Q_{\alpha\beta}\psi^\alpha\psi^\beta = 0$ for the quadric (cf. [53]). We assume that the quadric is nondegenerate in the sense that $\det(Q_{\alpha\beta}) \neq 0$. Then for any point $\xi^\alpha \in CP^3$ it follows that $\widetilde{\xi}_\alpha \triangleq Q_{\alpha\beta}\xi^\beta$ is nonvanishing. The locus consisting of all points ψ^α such that $\widetilde{\xi}_\alpha\psi^\alpha = 0$ defines the *polar plane* of the point ξ^α with respect to the quadric $Q_{\alpha\beta}$. Since $Q_{\alpha\beta}$ is nondegenerate, there is a unique inverse $Q^{\alpha\beta}$ satisfying $Q_{\alpha\gamma}Q^{\gamma\beta} = \delta_\alpha^\beta$, and thus for any plane η_α in CP^3 we can define a polar point $\widetilde{\eta}^\alpha \triangleq Q^{\alpha\beta}\eta_\beta$. The operation is involutory in the sense that the polar point of the polar plane of a given point is that point.

The polar plane of a point ξ can be constructed as follows. Let L be an arbitrary line through ξ. Then L intersects Q twice at, say, points A and B. Now suppose we consider the harmonic conjugate ξ^* of ξ, on the line L, with respect to the points A and B. This is the unique point ξ^* on L for which we have the cross-ratio $\{\xi, \xi^*; A, B\} = -1$. Then, as we vary L, the locus of ξ^* sweeps out a plane, and this is the polar plane $\widetilde{\xi}$. The polar plane $\widetilde{\xi}$ intersects Q in a conic $\mathcal{C}$ with the property that any line drawn from ξ to $\mathcal{C}$ touches Q tangentially. Conversely, if we consider all the lines through ξ that touch Q tangentially, then the union of the intersection points is the conic $\mathcal{C}$, which lies in a unique plane, the polar plane $\widetilde{\xi}$. A point lies on its polar plane iff the point itself lies on the quadric, in which case the polar plane of the point is the tangent plane at that point. In that case, the conic $\mathcal{C}$ degenerates into a pair of lines, given by the two generators of the quadric through the given point.

In the quantum mechanical situation we require further that the quadric $Q_{\alpha\beta}$ be Hermitian, or 'self-conjugate', in the sense that $Q_{\alpha\beta} = \bar{Q}_{\alpha\beta}$ and $Q^{\alpha\beta} = \bar{Q}^{\alpha\beta}$. This ensures that the complex conjugate ket-vector of the polar bra-vector $\widetilde{\zeta}_\alpha$ of a given ket-vector ζ^α agrees with the polar ket-vector of the complex conjugate bra-vector $\bar{\zeta}_\alpha$ of the given ket-vector ζ^α. It follows that complex conjugate ket-vector of the polar bra-vector of a disentangled state is also disentangled, and that the polar ket-vector of the complex conjugate bra-vector of a disentangled state is disentangled.

The geometry of a self-conjugate quadric applies to the consideration of any pair of two-state systems, whether or not these systems are of the same type. For example, we might consider a toy model in which a lepton is regarded as a composite consisting of a neutral spin $\frac{1}{2}$ particle and a spin 0 flavour doublet that determines whether the lepton is an electron or a muon. Then one might explore the properties of the entangled state given by a superposition of a spin-up electron with a spin-down muon, the spin state being given with respect to some choice of axis. What distinguishes the state space of a pair of spin $\frac{1}{2}$ particles is the existence of a preferred singlet state Z^α. This state is required to be self-conjugate polar with respect to the quadric in the sense that $\bar{Z}_\alpha = Q_{\alpha\beta}Z^\beta$.

We now present a geometrical construction for the supremum of the cross-ratio κ under the given constraint. Given the entangled state ψ^α we wish to find the state $X^\alpha \in Q$ that maximises the cross-ratio

$$\kappa = \frac{(\psi^\alpha\bar{X}_\alpha)(X^\beta\bar{\psi}_\beta)}{(\psi^\alpha\bar{\psi}_\alpha)(X^\beta\bar{X}_\beta)}.$$

Suppose we define $\bar{\psi}^\alpha \triangleq Q^{\alpha\beta}\bar{\psi}_\beta$, the polar state of the complex conjugate hyperplane $\bar{\psi}_\alpha$. Then we can show that the states on Q that are maximally and minimally distant to the

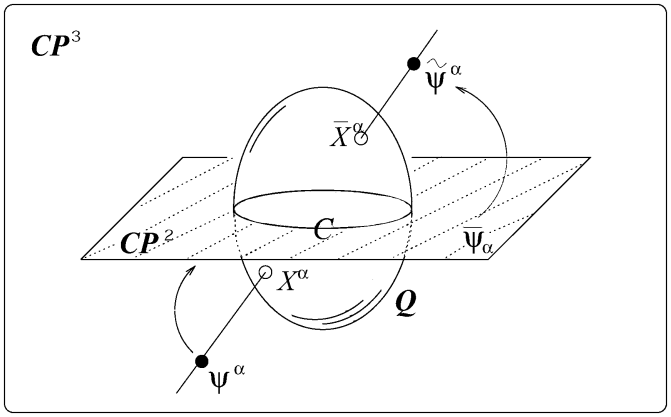

Fig. 9. *Construction of the nearest and furthest disentangled states*. Given any entangled state ψ^α we can form another state $\widetilde{\psi}^\alpha$ given by the complex conjugate of $\widetilde{\psi}_\alpha$, the polar conjugate plane of ψ^α with respect to the quadric Q. Providing that ψ^α is not maximally entangled, the points ψ^α and $\widetilde{\psi}^\alpha$ are distinct, and the points on Q closest to and furthest from ψ^α are given by the intersection points X^α and $\bar{X}^\alpha$ of Q with the line joining ψ^α and $\widetilde{\psi}^\alpha$.

given state ψ^α are collinear with ψ^α, and are complex conjugate polar to one another in the sense that ψ^α has to be of the form

$$\psi^\alpha = pX^\alpha + qQ^{\alpha\beta}\bar{X}_\beta,$$

where X^α is the point on Q closest to ψ^α, so $|p| \geq |q|$ (see Fig. 9). This can be verified, e.g., by maximising κ with respect to X^α subject to the constraint $Q_{\alpha\beta}X^\alpha X^\beta = 0$, using a Lagrange multiplier technique. Then if we define $\lambda = p/q$ it follows by a direct substitution that

$$\kappa = \frac{\lambda\bar{\lambda}}{1+\lambda\bar{\lambda}}.$$

Since $\lambda\bar{\lambda} \geq 1$, we deduce, further, that $\frac{1}{2} \leq \kappa \leq 1$. On the other hand, we can also verify by direct substitution that the invariant ρ defined by

$$\rho = \frac{(Q_{\alpha\beta}\psi^\alpha\psi^\beta)(\bar{Q}^{\gamma\delta}\bar{\psi}_\gamma\bar{\psi}_\delta)}{(\psi^\gamma\bar{\psi}_\gamma)^2},$$

which is independent of the scale of $Q_{\alpha\beta}$, depends on p and q only through λ, and is given by the formula

$$\rho = \frac{4\lambda\bar{\lambda}}{(1+\lambda\bar{\lambda})^2}.$$

Then it is not difficult to see that κ is indeed of the desired form $\kappa = \frac{1}{2}(1+\gamma)$ with $\gamma = \sqrt{1-\rho}$. That establishes the the validity of the expression indicated earlier for the minimum distance $\Delta = \cos^{-1}\gamma$ from the given state ψ^α to the quadric of disentanglement.

Suppose we consider the case of sub-maximally entangled states. In this situation the relation between ψ^α and X^α is invertible, since providing $|\lambda| > 1$ there exist complex

numbers r and s such that

$$X^\alpha = r\psi^\alpha + sQ^{\alpha\beta}\bar{\psi}_\beta.$$

We can solve this for the ratio $\mu = r/s$ by imposing the condition $Q_{\alpha\beta}X^\alpha X^\beta = 0$, leading to the quadratic equation $\mu^2 Q_{\alpha\beta}\psi^\alpha\psi^\beta + 2\mu\psi^\alpha\bar{\psi}_\alpha + \bar{Q}^{\alpha\beta}\bar{\psi}_\alpha\bar{\psi}_\beta = 0$, for which the roots are given by

$$\mu = \frac{-1 \pm \sqrt{1 - q\bar{q}}}{q},$$

where $q \triangleq Q_{\alpha\beta}\psi^\alpha\psi^\beta/\psi^\gamma\bar{\psi}_\gamma$. The positive root gives the point on Q nearest to ψ, and the negative root gives the most distant disentangled state, as illustrated in Fig. 9. We note that the terms here are so constructed that the solution for X^α is independent of the overall scale and phase of ψ^α, as expected.

The *maximally* entangled states are those for which $|\lambda| = 1$, for which apart from an overall irrelevant scale factor ψ^α is thus necessarily of the form

$$\psi^\alpha = \mathrm{e}^{\mathrm{i}\theta}X^\alpha + \mathrm{e}^{-\mathrm{i}\theta}Q^{\alpha\beta}\bar{X}_\beta.$$

Such states are self-conjugate in the sense that $\bar{\psi}_\alpha = Q_{\alpha\beta}\psi^\beta$. Conversely, given any disentangled state X^α we see that there exists a one-parameter family of maximally entangled states at a distance $\pi/2$ from it. This one-parameter family is given by the equatorial circle of the complex projective line obtained by joining X^α to the conjugate disentangled state $Q^{\alpha\beta}\bar{X}_\beta$, to which X^α is orthogonal.

Thus, e.g., if $X^{AB} = \xi^A\eta^B$ is a disentangled state of two spin $\frac{1}{2}$ particles, then we obtain the one-parameter family of maximally entangled states given by $\psi^{AB} = \mathrm{e}^{\mathrm{i}\theta}\xi^A\eta^B + \mathrm{e}^{-\mathrm{i}\theta}\bar{\xi}^A\bar{\eta}^B$, where $\bar{\xi}^A \triangleq \epsilon^{AB}\bar{\xi}_B$ and $\bar{\eta}^B \triangleq \epsilon^{BA}\bar{\eta}_A$. For any value of θ these states are at a distance of $\pi/2$ from X^{AB}.

A special case of interest arises when $\eta^B = \bar{\xi}^B$ and $\bar{\eta}^A = -\xi^A$. In that case, reverting to the notation of the previous section, we have $\psi^{AB} = \mathrm{e}^{\mathrm{i}\theta}\psi^A\bar{\psi}^B - \mathrm{e}^{-\mathrm{i}\theta}\bar{\psi}^A\psi^B$. Then for $\theta = 0$ we obtain the spin 0 singlet state for which $\psi^{AB} \propto \epsilon^{AB}$; whereas for $\theta = \pi$ we get the $S_z = 0$ spin 1 triplet state for which $\psi^{AB} \propto \psi^{(A}\bar{\psi}^{B)}$ (see Fig. 10).

More generally, if ψ^α is an *arbitrary* maximally entangled state, then consider the conic $\mathcal{K}$ that arises when we intersect the plane $\bar{\psi}_\alpha$ with the quadric Q. This conic is conjugate self-polar in the sense that for any point π^α on $\mathcal{K}$ the complex conjugate plane $\bar{\pi}_\alpha$ is tangent to the quadric at a point $\bar{\pi}^\alpha$ on $\mathcal{K}$. Now, suppose we consider the locus $\mathcal{L}$ of points generated by the intersection of the tangent lines to $\mathcal{K}$ at π^α and $\bar{\pi}^\alpha$ in the plane $\bar{\psi}_\alpha$ as we vary π^α. For any point P in $\mathcal{L}$ the join of that point with ψ^α intersects Q in a pair of points X^α and $\bar{X}^\alpha$, both of which are at a distance $\Delta = \pi/2$. By varying P we obtain all points on Q at a distance $\pi/2$ from ψ^α.

11. Schrödinger evolution

As the examples above indicate, the geometry of quantum mechanics is very rich, once specific physical systems are brought into play, even when there are only a few degrees

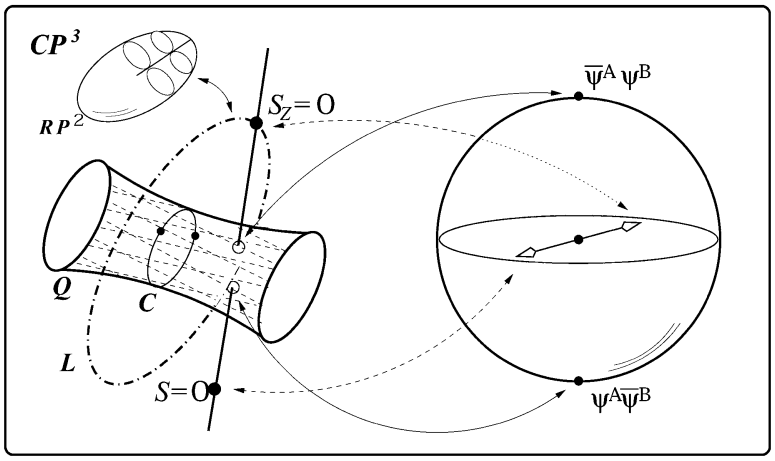

Fig. 10. *Maximally entangled states*. The $S = 0$ singlet and an $S_z = 0$ triplet state for some choice of z-axis are joined by a complex projective line that intersects Q in a pair of disentangled states. The singlet and triplet states lie on an equatorial circle at a distance of $\pi/2$ from the disentangled states which are orthogonal to one another and thus lie on opposite poles. All the points on this equatorial circle are maximally entangled. The locus L of the entangled triplet states corresponding to different spatial directions is topologically equivalent to a sphere with opposite points identified, i.e., RP^2. The conic C on Q, which has the topology of a sphere S^2, is the covering space of this locus. Hence the space of maximally entangled states thus constructed has a cone-like structure, obtained by joining each point of L to the unique singlet state $S = 0$, the join in each case being given by the corresponding equatorial circle.

of freedom. This picture can be further developed by consideration of the dynamics of a quantum system, which can be pictured as a vector field on the state manifold. Such a vector field generates a symmetry of the Fubini–Study geometry, i.e., an action of the projective unitary group.

In the case of an $(n + 1)$-dimensional Hilbert space, the state space is CP^n, which can be viewed as a real manifold Γ of dimension $2n$, with a symmetry group generated by a family of $n(n + 2)$ Killing vector fields. The generic Killing field on Γ has $n + 1$ fixed points, corresponding to the eigenstates of a nondegenerate Hamiltonian.

In the case of a two-dimensional Hilbert space, the state space is CP^1, and the specification of a Killing field selects out a pair of polar points on S^2, corresponding to energy eigenstates E_0 and E_1. The relevant symmetry is then given by a rigid rotational flow about this axis, the angular frequency being determined by Planck's formula $E_1 - E_0 = \hbar\omega$. For a general state space CP^n, in the generic situation, where the Hamiltonian is nondegenerate, with $n + 1$ distinct eigenvalues, the $n + 1$ fixed points of the given Killing field are linked by a figure consisting of $\frac{1}{2}n(n+1)$ spheres, for which the fixed points act as polar points, in pairs. These fixed points form the vertices of a regular simplex in CP^n, and under the action of the Killing flow the spheres linking these vertices rotate respectively with the characteristic angular frequencies

$$E_i - E_j = \hbar\omega_{ij},$$

where E_i ($i = 0, 1, \ldots, n$) labels the energy of ith eigenstate. The dynamical trajectories in Γ are determined by the specification of the fixed points, along with the associated angular frequencies. Even in the case of a simple spin 1 system, the geometry of the state space is intricate, given by a four-dimensional real manifold containing a system of three 2-spheres touching one another at the poles, and spinning at three distinct frequencies.

If the frequencies are incommensurate, i.e., not rational multiples of each other, then the Killing orbits do not close except on the three special spheres, and the generic dynamical trajectory, starting from some initial point in the state space, is doomed to evolve to eternity without ever returning to its origin. This raises the interesting question of whether the quantum trajectories exhibit some sort of ergodic property on the state space.

12. Quantum energy surfaces

In order to pursue this question further, let us consider the foliation of the $2n$-dimensional manifold Γ^{2n} by level surfaces of constant energy. The 'energy' here is given by the expectation of the Hamiltonian operator. For simplicity we consider here, specifically, the case of a nondegenerate Hamiltonian with eigenvalues E_i ($i = 0, 1, 2, \ldots, n$). The foliation corresponding to such a Hamiltonian contains two degenerate folia, associated with the extremal eigenvalues E_0 and E_n, for which the energy surfaces reduce to points. For values of E such that $E_0 < E < E_1$ or $E_{n-1} < E < E_n$, the energy surfaces are topologically equivalent to spheres S^{2n-1} of dimension $2n - 1$, endowed with a Riemannian geometry induced by the Fubini–Study metric.

For intermediate values of the energy, the resulting surfaces are more intricate, and are best perhaps considered on a case by case basis. If $0 < j < n$, then for $E_j < E < E_{j+1}$, the resulting manifold is given by a hyperboloid in $\mathbb{R}^{2n}$ of a certain signature, compactified by some spherical structure at infinity. The signature is given by $\{2(n-j), 2j\}$ for $0 < j < \frac{1}{2}n$, and by $\{2(j+1), 2(n-j-1)\}$ for $\frac{1}{2}n \leq j < n$. The intrinsic Riemannian structures of these surfaces, as well as the extrinsic embedding curvature, depend on the ratios of the energy differences $(E_i - E)/(E_j - E)$ for $i, j = 0, 1, \ldots, n$.

When E takes an eigenvalue E_k, the energy surface is singular at the point $\mathfrak{p}_k$ corresponding to the eigenstate with that eigenvalue. Thus, as E is increased we obtain a remarkable parametric family of manifolds punctuated by singular configurations, corresponding to the passage of E through its eigenvalues. In particular, the topological structure of the energy surface changes as E is increased from E_0 to E_n. We can view each of the structures thus arising as the topological phase associated with the given energy level E. If we also include the singular surfaces at the eigenvalues as different topological phases, then for a generic nondegenerate Hamiltonian with $(n + 1)$ eigenvalues, the energy folia admits n distinct topological phases.

For a Schrödinger evolution, the energy is clearly conserved, corresponding to the fact that the Killing trajectory associated with a given Hamiltonian necessarily lies in a level surface of that Hamiltonian. It follows, furthermore, that the resulting flow on a given such surface is an isometry of the Riemannian metric induced on that surface. Given an initial

state on a generic energy surface, the Killing trajectory is necessarily confined to a subfolium of dimension n that is topologically an n-torus T^n. The Killing trajectories that do not close thus exhibit a quasi-ergodic property on these toroidal subfolia.

Consider, e.g., the case of CP^2, for which the underlying geometry is already quite sophisticated (cf. [45]). Let us write ψ^α for a generic point and Z_i^α $(i = 0, 1, 2)$ for the eigenstates of a nondegenerate Hamiltonian, and E_i $(i = 0, 1, 2)$ for the corresponding eigenvalues, in ascending order. Then for the energy surface with energy E we have

$$E = \frac{E_0\psi_0\bar{\psi}_0 + E_1\psi_1\bar{\psi}_1 + E_2\psi_2\bar{\psi}_2}{\psi_0\bar{\psi}_0 + \psi_1\bar{\psi}_1 + \psi_2\bar{\psi}_2},$$

where $\psi_i \triangleq \psi^\alpha \bar{Z}_{i\alpha}$ and $\bar{\psi}_i \triangleq \bar{\psi}_\alpha Z_i^\alpha$ are the components of ψ^α and $\bar{\psi}_\alpha$, respectively, in a basis determined by the energy eigenstates Z_i^α $(i = 0, 1, 2)$.

Suppose that the energy E lies in the range $E_1 < E < E_2$. Then the equation for the energy surface can be rearranged in the form $(E - E_0)\psi_0\bar{\psi}_0 + (E - E_1)\psi_1\bar{\psi}_1 = (E_2 - E)\psi_2\bar{\psi}_2$. Because $E - E_0$ and $E - E_1$ are both by assumption positive, and because ψ_0 and ψ_1 cannot both be zero, it follows that the relevant energy surface necessary lies in the region of CP^2 such that $\psi_2 \neq 0$, i.e., an open region topologically equivalent to $\mathbb{R}^4$. As a consequence we can divide by ψ_2 to obtain

$$\frac{E - E_0}{E_2 - E}\alpha\bar{\alpha} + \frac{E - E_1}{E_2 - E}\beta\bar{\beta} = 1,$$

where $\alpha = \psi_0/\psi_2$ and $\beta = \psi_1/\psi_2$. The resulting energy surface is thus topologically a 3-sphere, and is given explicitly by a 3-ellipsoid in the $\mathbb{R}^4$ geometry coordinatised by the complex pair α, β.

Now we are able to consider more explicitly the Schrödinger trajectories, which in this example are given by

$$\alpha(t) = \mathrm{e}^{\mathrm{i}\hbar(E_0 - E_2)t}\alpha_0, \qquad \beta(t) = \mathrm{e}^{\mathrm{i}\hbar(E_1 - E_2)t}\beta_0$$

and thus generate a toroidal submanifold of the given 3-surface, provided both α_0 and β_0 are nonvanishing. Furthermore, the resulting family of toroidal surfaces can be parameterised by $|\alpha|$, which lies in the range $0 < |\alpha| < (E_2 - E)/(E - E_0)$. The limiting values of this range correspond to degenerate tori (circles); this situation arises when the initial state is orthogonal either to Z_0^α or Z_1^α, because the resulting Schrödinger evolution is necessarily confined to the projective line.

When $E = E_1$, the system is either in its eigenstate $\mathfrak{p}_1$, where $\psi_0 = \psi_2 = 0$, or otherwise we have $(E_1 - E_0)\psi_0\bar{\psi}_0 = (E_2 - E_1)\psi_2\bar{\psi}_2$ and ψ_1 arbitrary. In the latter case ψ_0 and ψ_2 are both necessarily nonvanishing, and we can divide by ψ_2 to obtain

$$\frac{E_1 - E_0}{E_2 - E_1}\alpha\bar{\alpha} = 1.$$

This determines a circle S^1, while the arbitrariness of ψ_1 implies that β can be written in the form $\beta = r\,\mathrm{e}^{\mathrm{i}\phi}$ for some real r and ϕ. Thus the energy surface associated with $E = E_1$

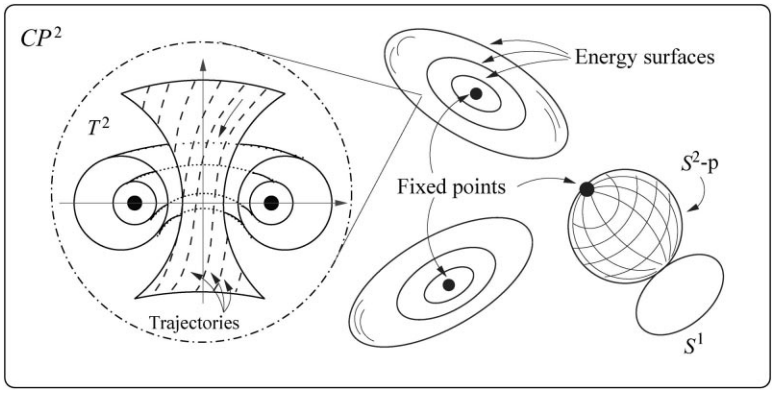

Fig. 11. *Foliation of the state space CP^2 by energy surfaces*. The quantum state space Γ is foliated by level surfaces of the expectation of the Hamiltonian operator. The Schrödinger evolution preserves the energy of a given initial state, and the resulting dynamical trajectory is confined to an n-torus T^n. If the ratios E_i/E_j of the energy eigenvalues are irrational, then the trajectory on T^n does not close. Here we illustrate the example of CP^2. In the case of a generic surface associated with the energy levels $E_0 < E < E_1$ and $E_1 < E < E_2$, the surfaces are 3-ellipsoids, while for $E = E_1$ the surface has a conical singularity at the eigenstate $\mathfrak{p}_1$.

is singular, and can be viewed as a cone $\mathcal{K}^3$ with the structure $\mathcal{K}^3 = (S^1 \times \mathbb{R}^2) + \mathfrak{p}_1$, where $\mathfrak{p}_1$ is the singular point.

In particular, if we take the complex projective line joining the extremal eigenstates $\mathfrak{p}_0$ and $\mathfrak{p}_2$, then there is a special circle on this projective line containing states for which the expected energy is the same as the eigenvalue E_1. Then the entire energy surface for $E = E_1$ is obtained by joining each point on this special circle to the point $\mathfrak{p}_1$. The joins thus obtained are each topological spheres, with a common intersection at $\mathfrak{p}_1$. If we delete $\mathfrak{p}_1$, then the punctured spheres separate, and we are left with the product $S^1 \times \mathbb{R}^2$. The topology change of the energy surface, as E evolves from E_0 to E_2, therefore, can be conveniently expressed as a topological sequence of the form

$$\mathfrak{p} \to S^3 \to S^1 \times \mathbb{R}^2 + \mathfrak{p} \to S^3 \to \mathfrak{p},$$

where $\mathfrak{p}$ denotes a point. This situation is illustrated in Fig. 11.

The situation in higher dimensions is rather more elaborate, but can be pursued by essentially the same kind of reasoning. It is worth noting that the role of the energy surfaces is significant in quantum statistical mechanics, and that the points raised above may thus be of relevance in that context as well.

13. Quantum Hamiltonian dynamics

This line of argument can be taken further by studying the quantum trajectories on Γ by use of differential geometry. When viewed as a real manifold, the state space is endowed with a Riemannian structure, given by a positive definite symmetric metric g_{ab}, a symplectic

structure, given by an antisymmetric tensor Ω_{ab}, and a complex structure, given by a tensor J^a_b, satisfying

$$J^a_c J^c_b = -\delta^a_b.$$

These structures are required to be *compatible* in the sense that $\Omega_{ab} = g_{ac} J^c_b$ and $\nabla_a J^b_c = 0$, where ∇_a is the covariant derivative associated with g_{ab}. Here we use Roman indices $(a, b, \dots)$ for tensorial operations in the tangent space of Γ. The compatibility of g_{ab}, Ω_{ab} and J^a_b makes Γ a Kähler manifold. The existence of a Hamiltonian structure on the Hilbert space $\mathcal{H}$ was pointed out by Chernoff and Marsden [31]. In the infinite-dimensional case it suffices, for some purposes, to make use of the fact that the metric g_{ab} and the symplectic structure Ω_{ab} are at least *weakly* nondegenerate in the sense that for any vector fields ξ^a, η^a on Γ, $\xi^a g_{ab} = 0$ implies $\xi^a = 0$ and $\eta^a \Omega_{ab} = 0$ implies $\eta^a = 0$. The fact that in infinite dimensions the Fubini–Study metric and symplectic structure are *strongly* nondegenerate [60] means that many of the geometrical constructions valid in finite dimensions carry through to the general quantum phase space.

The additional ingredient required for the specification of the dynamics is a Hamiltonian function $H(x)$ on Γ. Then the general dynamical trajectories on Γ are determined by a relation of the form

$$\tfrac{1}{2}\hbar \Omega_{ab}\, \mathrm{d}x^b = \nabla_a H\, \mathrm{d}t.$$

The Schrödinger trajectories on Γ are given by a subclass of the general Hamiltonian trajectories, namely, those for which the Hamiltonian function $H(x)$ is of the special quantum mechanical form

$$H(x) = \frac{\bar{\psi}_\alpha(x) H^\alpha_\beta \psi^\beta(x)}{\bar{\psi}_\gamma(x)\psi^\gamma(x)}.$$

Here, as before, $\psi^\alpha(x)$ denotes a set of homogeneous coordinates for the corresponding point x in the projective Hilbert space. We see that for a Schrödinger trajectory, $H(x)$ is the expectation of the Hamiltonian operator in the pure state to which the point x corresponds. In contrast with classical mechanics, where the phase space typically has an interpretation in terms of position and momentum variables, in quantum mechanics the points in phase space correspond to pure quantum states.

Quantum observables are intimately related to the metrical geometry of Γ. The distinguishing feature of a quantum Hamiltonian function $H(x)$ is that the associated symplectic gradient flow $\xi^a = \mathrm{d}x^a/\mathrm{d}t$ is a Killing field, i.e., $\nabla_{(a}\xi_{b)} = 0$. Indeed all Killing fields on Γ arise in this way through quantum observables. It is important to note that the Killing flows on Γ are necessarily Hamiltonian (cf. [66]). The Killing fields generate the symmetries of the Fubini–Study metric g_{ab}.

In the case of finite dimensions, we can say more about the quantum observables that generate isometries on the Fubini–Study manifold. If $H(x)$ corresponds to a standard linear observable, then in finite dimensions it is necessarily defined globally on Γ. One can show that such functions correspond to global solutions of the characteristic equation

$$\nabla^2 H = (n+1)(\bar{H} - H),$$

where ∇^2 is the Laplace–Beltrami operator on Γ, $\bar{H} = H^\alpha_\alpha/(n+1)$ is the uniform average of the eigenvalues of H^α_β, and $2n$ is the real dimension of Γ. Conversely, if we are given a Killing field ξ^a, the corresponding observable function $H(x)$ can be recovered, up to an additive constant, via the relation

$$\tfrac{1}{2}\hbar\Omega^{ab}\nabla_a\xi_b = (n+1)(H - \bar{H}),$$

which follows directly from the characteristic equation if we make use of the compatibility condition $g_{ab}\Omega^{ac}\Omega^{bd} = g^{cd}$ along with the fact that $\frac{1}{2}\hbar\xi_a = g_{ab}\Omega^{bc}\nabla_c H$. We note, incidentally, that in the Kibble–Weinberg theory, a general nonlinear quantum observable is a function on Γ such that the characteristic equation is *not* necessarily satisfied. As a consequence, the corresponding symplectic gradient flow is no longer necessarily a Killing field.

Now we are in a position to confirm the remark made in the previous section that the Schrödinger flow, when restricted to a given energy surface, will generate an isometry of that surface. This can be verified by showing that the Lie derivative

$$\mathcal{L}_\xi h_{ab} = \xi^c\nabla_c h_{ab} + h_{cb}\nabla_a\xi^c + h_{ac}\nabla_b\xi^c$$

vanishes, where $\frac{1}{2}\hbar\xi^a = \Omega^{ab}\nabla_b H$ is the Schrödinger flow and

$$h_{ab} = g_{ab} - \frac{\nabla_a H\nabla_b H}{\nabla_c H\nabla^c H}$$

is the induced metric on the given energy surface $H(x) = E$. A calculation then shows that the desired result follows as a consequence of the fact that ξ^a is a Killing vector of the Fubini–Study metric, and that the energy uncertainty is a constant of the motion along each Schrödinger trajectory.

14. Uncertainty relations and geometric phases

The metrical geometry of Γ also plays a significant role in determining the statistical properties of observables. For example, in the pure state x the squared uncertainty (variance) of a quantum mechanical observable represented by the function $F(x)$ is $(\Delta F)^2 = g_{ab}F^aF^b$, where F^a is the unique gradient vector field satisfying $g_{ab}F^b = \nabla_a F$. This leads to the following interpretation of quantum mechanical uncertainty. We foliate Γ with surfaces given by level values of $F(x)$. We allow the foliation to be 'singular' in places, e.g., at the energy eigenstates, where the energy surfaces are degenerate.

Through a given pure state x there is a unique such surface, and the uncertainty ΔF is the length of the gradient vector to that surface at x (see Fig. 12). The observables $F(x)$ and $G(x)$ are incompatible if their Poisson bracket $[F, G] = \Omega_{ab}F^aG^b$ is nonvanishing. In that case the Heisenberg uncertainty relation

$$(\Delta F)^2(\Delta G)^2 \geq \tfrac{1}{4}|[F, G]|^2$$

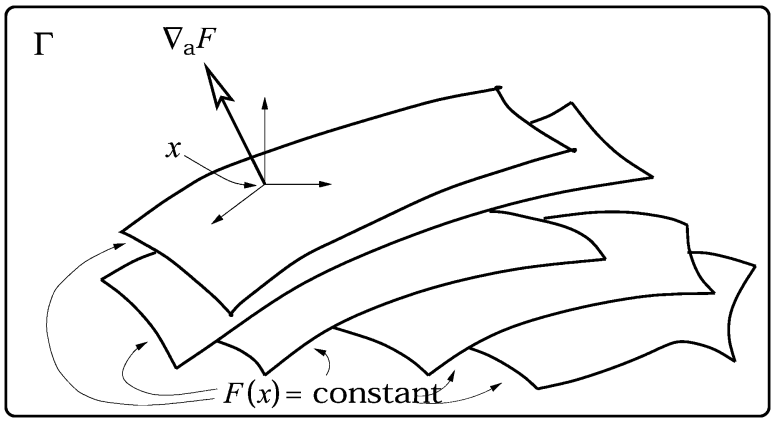

Fig. 12. *The observable uncertainty*. The quantum phase space Γ is foliated locally by level surfaces of the function $F(x)$. The quantum uncertainty in the corresponding observable, in the pure state x, is given by the magnitude of the gradient of $F(x)$ at that point.

follows directly as a consequence of the geometric inequality

$$(g_{ab}F^aF^b)(g_{ab}G^aG^b) \geq (g_{ab}F^aG^b)^2 + \tfrac{1}{4}(\Omega_{ab}F^aG^b)^2,$$

if we omit the first term in the right-hand side. This inequality, which follows as a consequence of the standard argument for the Hermitian Schwartz inequality in Hilbert space, holds for any vector fields F^a and G^a on a Kähler manifold. Note that the omitted term $g_{ab}F^aG^b$ gives rise to the anticommutator of the observables F and G.

The geometrical approach to uncertainty here ties in closely with the statistical idea of the Cramér–Rao inequality for the variance lower bound in estimation theory (cf. [49,80]). In the case of a pair of canonically conjugate observables $P(x)$ and $Q(x)$ defined on an appropriate region of Γ, satisfying $[P, Q] = \hbar$, we can expand the gradient to the surfaces of constant $Q(x)$ in a suitable basis to obtain a series of generalised Heisenberg relations [18–21], an example of which is

$$(\Delta P)^2(\Delta Q)^2 \geq \frac{1}{4}\hbar^2\left(1 + \frac{(\mu_4(P) - 3\mu_2(P)^2)^2}{\mu_6(P)\mu_2(P) - \mu_4(P)^2}\right),$$

where $\mu_k(P) = \langle(P - \langle P\rangle)^k\rangle$ is the kth central moment of the observable P in the state x. This inequality has the following statistical interpretation. Suppose that we are given an unknown quantum state of a particle, parameterised by its position q, and that we wish to estimate the position of the particle by a suitable measurement. The observable function corresponding to the parameter q is then given by Q, and the statistical estimation of q via measurement on Q gives rise to an inevitable variance lower bound, expressed in terms of a certain combination of the moments $\mu_k(P)$ of the momentum distribution associated with the given state. Likewise, if we consider momentum estimation, then the corresponding variance lower bound is given by the moments of the position Q.

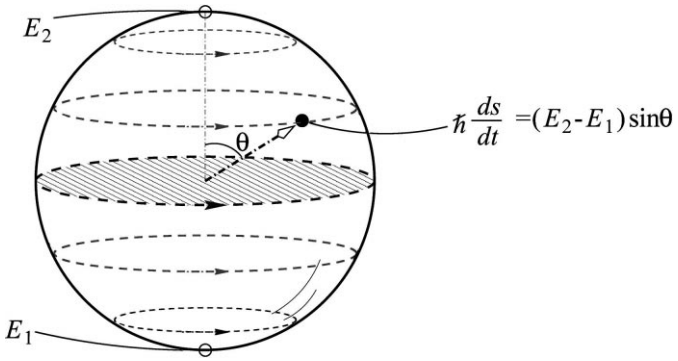

Fig. 13. *The Anandan–Aharonov relation*. The quantum evolution of a two-state system corresponds to the rigid rotation of a 2-sphere with angular frequency $\hbar\omega = E_2 - E_1$. The speed of the trajectory is greatest at the equator, which consists of states of maximal energy uncertainty.

An interesting interplay between the quantum dynamical trajectories and the uncertainty relations was pointed out by Anandan and Aharonov [8]. In particular, it follows from the projective Schrödinger equation $\frac{1}{2}\hbar\Omega_{ab}\,\mathrm{d}x^b = \nabla_a H\,\mathrm{d}t$ and the expression for the line element $\mathrm{d}s^2 = g_{ab}\,\mathrm{d}x^a\,\mathrm{d}x^b$ that the 'speed' in the state space Γ along the dynamical trajectory at the point x is

$$\frac{1}{2}\hbar\frac{\mathrm{d}s}{\mathrm{d}t} = \Delta H,$$

where ΔH is the energy uncertainty in the given state. For example, in the case of a two-state system with eigenstates at the poles of a 2-sphere, the quantum evolution corresponds to a rigid rotation of the sphere, with constant angular frequency, for which the speed is greatest at the equator, corresponding to states of maximum uncertainty (as shown in Fig. 13).

This result is related to properties of the *geometric phase* introduced by Berry and subsequently applied in many situations [6,7,15,84,86,89–93]. Consider a closed path γ in the quantum phase space. If γ is a standard dynamical trajectory, then it corresponds to a closed Killing orbit, but we shall allow for the possibility of more general paths, e.g., as might be generated by a time-dependent Hamiltonian operator. The geometric phase associated with such a cyclic evolution is given by the integral

$$\beta[\gamma] = \int_\Sigma \Omega_{ab}\,\mathrm{d}x^a \wedge \mathrm{d}x^b,$$

where Σ is any real 2-surface in Γ such that $\gamma = \partial\Sigma$. Owing to the relation $\nabla_a\Omega_{bc} = 0$, it follows from Stokes' theorem that the value of $\beta[\gamma]$ is independent of the choice of surface Σ spanning the loop γ, and can be given the following interpretation.

The punctured Hilbert space $\widetilde{\mathcal{H}} = \mathcal{H} - \{0\}$, with the origin deleted, is a fibre bundle over Γ. Therefore, given a trajectory γ in Γ, we can form a corresponding trajectory $\mathcal{P}^{-1}[\gamma]$

in $\widetilde{\mathcal{H}}$, called the horizontal lift of γ. This is obtained by solving the *modified* Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi^\alpha}{\partial t} = (H^\alpha_\beta - E[H]\delta^\alpha_\beta)\psi^\beta,$$

where $E[H]$ is the expectation of the Hamiltonian in the state ψ^α. Despite its nonlinearity, the modified Schrödinger equation is physically natural inasmuch as its stationary states are energy eigenstates. In this connection, it is worth drawing attention to the fact that in the case of the modified Schrödinger dynamics, the time-independent Schrödinger equation

$$H^\alpha_\beta\psi^\beta = E[H]\psi^\alpha$$

follows directly from the stationary state requirement, without the introduction of the so-called correspondence principle $E[H] \leftrightarrow \mathrm{i}\hbar\partial_t$.

The horizontal lift is characterised by the condition that the tangent to the curve $\mathcal{P}^{-1}[\gamma]$ in $\widetilde{\mathcal{H}}$, given by $\partial\psi^\alpha/\partial t$, is orthogonal to the fibre direction ψ^α, so we have $\bar{\psi}_\alpha\partial\psi^\alpha/\partial t = 0$.

In the case of a closed loop γ, $\beta[\gamma]$ measures the phase change in ψ^α over the corresponding circuit in $\mathcal{P}^{-1}[\gamma]$. If the given loop γ in Γ subsequently evolves in time, then $\beta[\gamma]$ is a quantum mechanical analogue of the Poincaré integral invariant (cf. [2,9]), as illustrated in Fig. 14. We note, incidentally, that the notion of geometric phase discussed here also applies to nonlinear quantum mechanics, for which the Hamiltonian $H(x)$ does

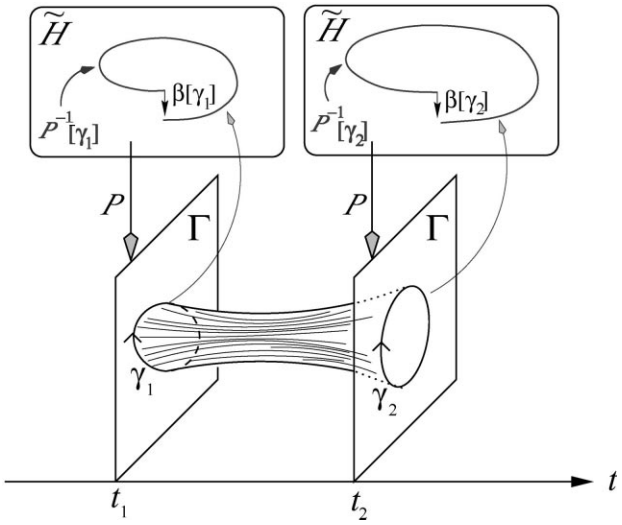

Fig. 14. *The horizontal lift of a quantum trajectory and Poincaré's invariant integral*. The Berry phase $\beta[\gamma]$ associated with a general cyclic trajectory γ in the quantum phase space Γ is given by the integral of the symplectic form Ω_{ab} over a 2-surface Σ spanning γ. This integral measures the phase change that develops in the horizontal lift of γ to the corresponding path $\mathcal{P}^{-1}[\gamma]$ in the Hilbert bundle $\widetilde{\mathcal{H}}$ over Γ. If the cyclic trajectory subsequently evolves unitarily in time, then $\beta[\gamma]$ is the quantum analogue of the integral invariant of Poincaré, and we have $\beta[\gamma_1] = \beta[\gamma_2]$. This result is valid even if we relax the unitarity condition and consider nonlinear dynamics of the Kibble–Weinberg type.

not satisfy the characteristic equation for linear observables. The role of the geometric phase in both linear and nonlinear quantum mechanics continues to be explored.

15. Mixed states

Phase-space geometry sheds some light on the peculiar role of probability in quantum mechanics. For a review of the current status of the relation between classical and quantum probability, see, e.g., [87]. For many purposes it suffices to characterise the state of a quantum system by its density matrix, which allows one to compute the expectation of any observable. The question is, is this sufficient for *all* purposes? In this connection we note that there are at least two situations where it is useful to consider probability distributions on the state manifold Γ itself. One is in the description of the statistical properties of a measurement outcome; the other is the representation of ensembles in quantum statistical mechanics.

In both cases, the state of the system can be characterised by a probability density function or measure $\rho(x)$ on Γ, in terms of which the expectation of any function $F(x)$ on Γ can be written

$$E[F] = \int_\Gamma \rho(x) F(x)\, \mathrm{d}x.$$

We think of $F(x)$ as representing the expectation of the corresponding (possibly nonlinear) observable, *conditional* on the system being in the pure state x. Then $E[F]$ is the *unconditional* expectation, where we average $F(x)$ over the pure states, weighting with the density $\rho(x)$. A pure state arises if $\rho(x)$ is a δ-function concentrated on a point in Γ. Consider the example of a measurement where initially the system is in a pure state X, and the observable has a finite number of eigenstates, as in the case of a spin 1 system when we measure the spin along an axis. The result of this measurement is one of the three spin eigenstates, and these arise with probabilities determined by the Fubini–Study distance. The density function $\rho(x)$ for the state of the system after a measurement is given by a sum of three δ-functions, concentrated at the eigenstates, weighted by these probabilities.

In the case of a *linear* quantum observable, the unconditional variance of $F(x)$ in a general mixed state $\rho(x)$ is given by

$$V[F] = \int_\Gamma \rho(x)(F(x) - E[F])^2\, \mathrm{d}x + \int_\Gamma \rho(x)(g_{ab} F^a F^b)^2\, \mathrm{d}x.$$

A further simplification emerges by virtue of the special form of a linear observable, for which we have $E[F] = \rho^\alpha_\beta F^\beta_\alpha$, where

$$\rho^\alpha_\beta = \int_\Gamma \rho(x) \frac{\bar{\psi}_\beta(x)\psi^\alpha(x)}{\bar{\psi}_\gamma(x)\psi^\gamma(x)} \mathrm{d}x$$

is the *density matrix* associated with $\rho(x)$. The infinite-dimensional analogue of this formula has been established by Cyranski [36]. For the calculation of expectations in ordinary linear

quantum mechanics it suffices to consider the density matrix alone, since all such statistical quantities calculated with $\rho(x)$ reduce to expressions involving ρ^α_β. Therefore, for certain purposes we can regard ρ^α_β itself as offering a complete representation of the state of the system. Indeed, a considerable literature now exists analysing various aspects of the geometry of the space of density matrices (see, e.g., [37,38,59,75,89–93], and references cited therein).

One should bear in mind, however, that the density matrix ρ^α_β, which is the lowest moment of the projection operator in the state $\rho(x)$, does not in general contain all the information of the system when we are dealing with nonlinear observables. This follows from the fact that the information of a generic state $\rho(x)$ is contained in the set of *all* the moments (cf. [25,63]). In the case of a nonlinear observable, we must consider a general state $\rho(x)$, pure or mixed, because the density matrix is not sufficient to take the expectation of such an observable. Some specific examples of nonlinear observables have been studied, e.g., by Weinberg [95,96]. The entanglement measure Δ introduced in Section 9 provides another interesting example of a nonlinear observable arising in a natural context. Indeed, now we are able to examine the issue of entanglement as it applies to mixed states. This is an area of investigation of considerable current interest (cf. [50,59], and references cited therein), and it has a natural characterisation in the geometrical approach. More specifically, given a general mixed state $\rho(x)$ on the quantum state space, the associated measure of entanglement is given by the expectation

$$\Delta(\rho) = \int_\Gamma \rho(x)\Delta(x)\,\mathrm{d}x,$$

which is invariant under local unitary transformations that preserve the disentangled state space. The exclusive consideration of the density matrix in a nonlinear setting can lead to paradoxical conclusions, such as the possibility of superluminal EPR communication (cf. [46,47,78]).

Given a general state $\rho(x,t)$ and a Hamiltonian $H(x)$, the evolution of $\rho(x,t)$ is governed by the Liouville equation,

$$\frac{1}{2}\hbar\frac{\partial\rho}{\partial t} = \Omega^{ab}\nabla_a\rho\nabla_b H,$$

where the Poisson bracket between $\rho(x,t)$ and $H(x)$ is determined by the symplectic structure Ω_{ab} on Γ. In the case where the Hamiltonian is a linear quantum observable, the Liouville equation is equivalent to the standard Schrödinger dynamics associated with a mixed state $\rho(x,t)$. On the other hand, if the Hamiltonian is a nonlinear observable, then the Liouville equation no longer corresponds to a linear Schrödinger evolution.

It is interesting to note, nevertheless, that, contrary to what has been argued in literature (cf. [74]), in the case of nonlinear quantum mechanics of the Kibble–Weinberg type, the quantum Shannon entropy

$$S(\rho) = -\int_\Gamma \rho(x,t)\ln\rho(x,t)\,dx$$

associated with a general mixed state $\rho(x,t)$ remains constant in time (cf. [97]). This result, which is insensitive to the specific functional form of $S(\rho)$, follows as a consequence of the Liouville equation for $\rho(x,t)$. One can also show [25] that, given the information of the density matrix ρ^α_β, the corresponding quantum Shannon entropy obtained by maximising $S(\rho)$ is generally different from the von Neuman entropy.

More generally, the definition of entropy and equilibrium in quantum statistical mechanics brings up conceptual issues, since, like the quantum measurement problem, it involves the interface of microscopic and macroscopic physics. There is also a relationship to fundamental issues in probability theory. Suppose we consider a quantum system characterised by a state space Γ and a Hamiltonian function $H(x)$ with discrete, possibly degenerate energy levels E_j ($j = 1, 2, \ldots, N$). Let us write $\delta_j(x)$ for a normalised δ-function on Γ concentrated on the pure state x_j with energy E_j. Thus, x_j is the jth energy eigenstate. Then if the quantum system is in equilibrium with a heat-bath at inverse temperature $\beta = 1/kT$, the state of the system is evidently of the form

$$\rho(x) = \frac{\sum_j \exp(-\beta E_j)\delta_j(x)}{Z(\beta)},$$

where $Z(\beta) = \sum_j \exp(-\beta E_j)$ is the partition function. This is the canonical distribution of quantum statistical mechanics, characterised by a Gibbs distribution concentrated on the energy eigenstates with Boltzmann weights $\exp(-\beta E_j)/Z(\beta)$. The standard canonical density matrix associated with this distribution is $\rho^\alpha_\gamma = \exp(-\beta H^\alpha_\gamma)/Z(\beta)$, which is clearly independent of the phase and scale of the underlying energy eigenvectors, and thus can be regarded as belonging to the geometry of Γ.

16. Quantum theory and beyond

There is an element of paradox at the heart of statistical mechanics, related to the fact that there are many distinct probability distributions on Γ that give rise to the canonical density matrix. A natural question to ask, therefore, is whether there exists a 'preferred' density function on Γ for the canonical ensemble. In the case of classical mechanics, the maximum entropy argument 'selects' a preferred distribution subject to the given constraints. It is interesting therefore that when applied to quantum mechanics, this argument leads to a quantum canonical ensemble characterised by the measure

$$\rho(x) = \frac{\exp(-\beta H(x))}{\int_\Gamma \exp(-\beta H(x))\,\mathrm{d}x}$$

rather than the system of weighted δ-functions concentrated on energy eigenstates indicated earlier [22,23]. However, the maximum entropy ensemble on Γ projects to a density matrix quite distinct from the canonical density matrix. It may be that in the limit of a large number of constituents there is an equivalence of ensembles, analogous to that arising in classical statistical mechanics. The point here is that, even if the macroscopic energy of a substance in thermal equilibrium with a fixed heat-bath is specified, there is no known

principle that requires the individual subconstituents of that substance to be in energy eigenstates. Could it be that in some situations there exists a mechanism that causes systems to spontaneously devolve to energy eigenstates? A promising example of such a mechanism is the energy-based stochastic state vector reduction process considered by Gisin [46], Percival [73], Hughston [52], and Adler and Horwitz [3].

A further reason for the consideration of general probability distributions on Γ is that such states are necessary for an account of the statistical properties of observables in nonlinear quantum systems. These systems were given a general characterisation by Kibble [55,56], who observed that if we keep the phase space Γ of quantum mechanics, along with the Fubini–Study metric and the associated symplectic structure, but extend the category of observables to include more general functions on Γ, then the corresponding nonlinear Schrödinger dynamics can still be expressed in Hamiltonian form, i.e., $\frac{1}{2}\hbar\Omega_{ab}\,\mathrm{d}x^b = \nabla_a H\,\mathrm{d}t$. Here $H(x)$ represents a general nonlinear functional of the wave function, not necessarily the expectation of a linear operator. The peculiar status of such functions in linear quantum mechanics was pointed out by Mielnik [63], who remarks, '... in the orthodox theory only the quadratic forms are observables: the other functions ... though they can be experimentally determined, are not statistical averages of any quantum mechanical experiment'.

An example of an evolution generated by a nonlinear observable is given by the Newton–Schrödinger equation. Consider a quantum system of self-gravitating particles, described by the Schrödinger equation in $\mathbb{R}^3$ with a potential $\phi(\mathbf{x})$, as described earlier, where $\phi(\mathbf{x})$ is the gravitational potential due to the probable mass distribution of the quantum system, given by the Poisson equation $\nabla^2\phi(\mathbf{x}) = 4\pi m p(\mathbf{x})$, where $p(\mathbf{x}) = \bar{\psi}(\mathbf{x})\psi(\mathbf{x})/\int \bar{\psi}(\mathbf{x})\psi(\mathbf{x})\,\mathrm{d}^3\mathbf{x}$. Because the potential depends on the wave function $\psi(\mathbf{x})$, the resulting Schrödinger equation is nonlinear. As another example of nonlinear dynamics we might envisage a modification of the Schrödinger equation that would tend to drive an initially entangled system towards a state of disentanglement.

The general features of phase space based nonlinear quantum dynamics have been studied by a number of authors (e.g., [3,42,46,51,52,57,64,65,73,74,78,95–97]). We also draw attention to the work of Bialynicki-Birula and Mycielski [16]. It is surprising how naturally geometric quantum mechanics can be adapted to so many aspects of the nonlinear regime. This suggests that the geometric approach may eventually be useful in solving some of the key open problems in quantum theory, e.g., a clear understanding of the process of state reduction and a proper integration of the theory with gravitation [13,39,98].

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