Geometry of Quantum Evolution

J. Anandan[(a)]
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 9EW, United Kingdom

Y. Aharonov[(b)]
Department of Physics and Astronomy, University of South Carolina, Columbia, South Carolina 29208
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For an arbitrary quantum evolution, it is shown that the integral of the uncertainty of energy with respect to time is independent of the particular Hamiltonian used to transport the quantum system along a given curve in the projective Hilbert space. It is the distance along this curve measured by the Fubini-Study metric. This gives a new time-energy uncertainty principle. New geometric meanings to time as measured by a clock and the transition probability during a quantum measurement are also obtained.

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It is well known that geometric ideas have played an important role in physics. For example, Minkowski's geometric reformulation of special relativity by means of a space-time geometry was very useful in the construction of general relativity by Einstein. But it may be fair to say that there was a lack of the geometric approach to quantum theory until Berry's remarkable discovery[1] that there is a geometric phase in the cyclic evolution of an adiabatically evolving system. This geometric phase was reformulated and generalized to nonadiabatic cyclic evolutions[2,3] by using the projective Hilbert space $\mathcal{P}$, which is defined as the set of rays of the Hilbert space $\mathcal{H}$. The geometric phase factor was obtained as the holonomy transformation or parallel transport around a closed curve with respect to the natural connection over $\mathcal{P}$ given by the inner product on the Hilbert space.[2,4,5] The geometric phase has also been interpreted as an area enclosed by the closed curve with respect to a natural symplectic structure in $\mathcal{P}$.[6] This approach has the advantage that, in addition to removing the restriction of adiabaticity, there is a nontrivial geometric phase even for a closed system for which the Hamiltonian is constant in time,[7] unlike in Berry's approach in which the Hamiltonian must vary with time.

In this Letter we shall develop a geometric approach towards *all* quantum evolutions, not merely cyclic evolutions. We assume that a quantum evolution of a state $|\psi(t)\rangle$ is governed by the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle=H(t)|\psi(t)\rangle\,, \tag{1}$$

where H is the Hamiltonian. For an isolated system to move in $\mathcal{P}$, it is necessary and sufficient that it is not a stationary state, i.e., it has a nonzero value for the uncertainty $\Delta E(t)$ in energy defined by

$$\Delta E^2=\langle\psi|H^2|\psi\rangle-\langle\psi|H|\psi\rangle^2\,. \tag{2}$$

We shall now consider the most general case when H may depend on t and show that the quantity

$$s=2\int\frac{\Delta E(t)}{\hbar}dt \tag{3}$$

is independent of the particular $H(t)$ used to transport the state along a given curve C in $\mathcal{P}$. Hence it is a geometric quantity analogous to the geometric phase[2] and is in fact the distance along C as measured by the Fubini-Study metric[5,8] which is defined naturally from the inner product in Hilbert space.

To prove this, Taylor expand $|\psi(t+dt)\rangle$ to second order in dt, and use (1) and its time derivative:

$$|\psi(t+dt)\rangle=|\psi(t)\rangle-\frac{idt}{\hbar}H|\psi(t)\rangle-\frac{dt^2}{2\hbar}\left(i\frac{dH}{dt}|\psi(t)\rangle+\frac{1}{\hbar}H^2|\psi(t)\rangle\right)+O(dt^3)\,. \tag{4}$$

Since H is Hermitian, so is dH/dt and H^2. Then, on using (2),

$$|\langle\psi(t)|\psi(t+dt)\rangle|^2=1-\frac{dt^2\Delta E^2}{\hbar^2}+O(dt^3)\,. \tag{5}$$

Therefore, $\Delta E\,dt/\hbar$ is independent of the phases of $|\psi(t)\rangle$ and $|\psi(t+dt)\rangle$ and therefore depends only on the points in $\mathcal{P}$ to which they project. There are infinite number of Hamiltonians which would evolve the state along a given curve C in $\mathcal{P}$. In general, they give rise to different phase factors for the state vector. But they all give the same value for the dimensionless quantity s defined by (3). Since s is independent of the particular Hamiltonian used to achieve the motion, we expect it to have a geometric meaning analogous to the geometric phase[2] for closed curves in $\mathcal{P}$.

To investigate the meaning of s we introduce some geometric concepts. Suppose $\mathcal{H}$ has dimension $N+1$ where N is a non-negative integer or infinity. The unitary group $U(N+1)$ acting on $\mathcal{H}=\mathcal{C}^{N+1}$ can be identified with the set $\mathcal{B}$ of orthonormal bases of $\mathcal{H}$ because each element of $\mathcal{B}$ can be obtained from a fixed element of $\mathcal{B}$ by the action of a unique element of

$U(N+1)$. On defining an equivalence relation between two orthonormal bases whenever the first element of both bases is the same, the corresponding quotient set of $\mathcal{B}$, which is the same as $U(N+1)/U(N)$, may be identified with the set of unit vectors of $\mathcal{H}$ and is called a Stiefel manifold S_N. The equivalence relation on S_N identifying any two unit vectors related by multiplication by a phase factor gives the quotient set $U(N+1)/U(N)\times U(1)$ which can be identified with $\mathcal{P}=P_N(\mathcal{C})$, i.e., the N-dimensional complex projective space. Now, $U(N+1)$ is a principal fiber bundle over S_N with projection map Φ (say) and structure group $U(N)$. Also, S_N is a principal fiber bundle over $\mathcal{P}$ with projection map Π (say) and structure group $U(1)$, which is sometimes called the Hopf bundle. Also, $U(N+1)$ may be regarded as a principal fiber bundle over $\mathcal{P}$ with projection map $\Pi\Phi$ and structure group $U(N)\times U(1)$.

There are natural metrics on the above bundles defined as follows: A tangent vector X of $U(N+1)$ is a $(N+1)$-dimensional Hermitian matrix. Define the metric h in $\mathcal{B}$ by the condition $h(X,Y)=2\,\mathrm{tr}(XY)$, where X and Y are tangent vectors at any point in $\mathcal{B}=U(N+1)$, assuming for the present that N is finite. It is easily verified that this metric is real and positive definite and when restricted to the $SU(N+1)$ subgroup it is the Cartan-Killing metric. Let g be the metric in S_N such that Φ is a Riemannian submersion, i.e., $d\Phi$ is an isometry when restricted to the orthogonal complement of the kernel of $d\Phi$. Similarly, define a metric f on $\mathcal{P}$ such that Π is a Riemannian submersion. This f is the *Fubini-Study metric*. There are now natural connections on each of the three bundles defined as follows: The horizontal space at each point is orthogonal to the fiber at that point with respect to the metric in that bundle. The geometric phase factor[2] $e^{i\beta}$ is obtained as the parallel transport around a closed curve of $\mathcal{P}$, with respect to the connection in S_N.

We now obtain an expression for the Fubini-Study metric directly in terms of representative state vectors of points in $\mathcal{P}$. Let $|\psi_1\rangle$ and $|\phi\rangle$ be two arbitrary normalized vectors in $\mathcal{H}$. Extend $|\psi_1\rangle$ to an orthonormal basis $\{|\psi_a\rangle,\ a=1,2,\ldots,N+1\}\in\mathcal{B}$ such that $|\phi\rangle=\cos(\frac{1}{2}\theta)|\psi_1\rangle+\sin(\frac{1}{2}\theta)|\psi_2\rangle$, $\theta\in[0,2\pi]$. Now, the curve in $\mathcal{B}$ through this basis defined by $s\to\exp(isK)|\psi_a\rangle$, where the only nonzero elements of K in this basis are $\langle\psi_2|K|\psi_1\rangle=\langle\psi_1|K|\psi_2\rangle=\frac{1}{2}$, is a horizontal geodesic in $\mathcal{B}$ with s being the distance along this curve as measured by the metric h. Therefore, this curve projects to a geodesic in $\mathcal{P}$ with s now being the distance measured by the Fubini-Study metric f. Clearly, this geodesic is a closed curve of total length 2π. Since, $|\phi\rangle=\exp(isK)|\psi_1\rangle$ when $s=\theta$, $\Pi(|\psi_1\rangle)$ and $\Pi(|\phi\rangle)$ are points in $\mathcal{P}$ which lie on this geodesic separated by the distance θ. If $|\psi\rangle$ is $|\psi_1\rangle$ multiplied by an arbitrary phase factor, then

$$|\langle\psi|\phi\rangle|^2=\cos^2(\tfrac{1}{2}\theta)\,. \qquad (6)$$

When $\theta\neq 0$, $|\psi\rangle$ and $|\phi\rangle$ span a two-dimensional subspace $\mathcal{C}^2$ of $\mathcal{H}$. The set of rays of $\mathcal{C}^2$ is the complex one-dimensional projective space $P_1(\mathcal{C})$, which is also a real two-dimensional sphere and a submanifold of $\mathcal{P}$. The Fubini-Study metric when restricted to this sphere is the usual metric on a sphere with unit radius. Every geodesic joining $\Pi(|\psi\rangle)$ and $\Pi(|\phi\rangle)$ is a projection of a horizontal geodesic in $\mathcal{B}$, which can be written in the above form by an appropriate choice of basis. Therefore it must lie on this sphere. If $\theta\neq\pi$, then there are exactly two geodesics joining $\Pi(|\psi\rangle)$ and $\Pi(|\phi\rangle)$ which together form a great circle on this sphere. If $\theta=\pi$, corresponding to $|\psi\rangle$ and $|\phi\rangle$ being orthogonal, there are infinite number of geodesics with the same length joining $\Pi(|\psi\rangle)$ and $\Pi(|\phi\rangle)$, which are opposite points on the sphere. The normalization of our metrics was chosen so that (6) is valid for any geodesic joining these two points for arbitrary states $|\psi\rangle$ and $|\phi\rangle$.

We therefore conclude that *the probability of transition* $|\langle\psi|\phi\rangle|^2$ *between any two states* satisfies (6), where θ is the distance along any geodesic joining $\Pi(|\psi\rangle)$ and $\Pi(|\phi\rangle)$. Thus, the result of every measurement made on a quantum system in the laboratory has this geometric meaning. In particular, consider the filtering measurements studied by Pancharatnam[9] by sending light through a sequence of polarizers, which provided the first known example of the geometric phase.[10,11] In such a measurement a state undergoes the transition $|\psi\rangle\to|\phi\rangle\langle\phi|\psi\rangle$. The new state has a well-defined phase and has undergone a fractional reduction of intensity $|\langle\psi|\phi\rangle|^2$. The phase can be determined by the theorem[3,11,12] which states that the new state can be obtained by parallel transporting $|\psi\rangle$ along the *shortest* geodesic joining $\Pi(|\psi\rangle)$ and $\Pi(|\phi\rangle)$ in $\mathcal{P}$ and multiplying by the non-negative number $|\langle\psi|\phi\rangle|$. But we now also have a geometric interpretation for this number as $\cos(\frac{1}{2}\theta)$, where $\theta\in[0,\pi]$ is the distance along this geodesic segment.

Suppose that $|\psi\rangle$ and $|\psi'\rangle=|\phi\rangle$ are such that $\Pi(|\psi\rangle)$ and $\Pi(|\psi'\rangle)$ are separated by an infinitesimal distance. Then, setting $ds=\theta$ in (6), we obtain the following expression for the Fubini-Study metric $g_{\mu\bar{\nu}}$:

$$ds^2=2g_{\mu\bar{\nu}}dZ^\mu d\bar{Z}^\nu=4(1-|\langle\psi|\psi'\rangle|^2)\,, \qquad (7)$$

where Z^μ are coordinates in $\mathcal{P}$.[13] Equation (7) may be regarded as an alternative definition of the Fubini-Study metric. Clearly, this definition is valid also for an infinite-dimensional $\mathcal{H}$. A unitary or antiunitary transformation leaves $|\langle\psi|\psi'\rangle|$ invariant and is therefore an isometry in $\mathcal{P}$. Hence *the unitary time evolution (1) and all unitary and antiunitary symmetries in* $\mathcal{H}$ *are isometries in* $\mathcal{P}$. It may be noted that while symmetries such as rotations and Galilei boosts have a projective representation in $\mathcal{H}$, they always have a faithful representation in $\mathcal{P}$. For example, the rotation of fermion wave functions by 2π rad results in a sign change in $\mathcal{H}$, but the corresponding isometry in $\mathcal{P}$ is the identity.

From (5) and (7),

$$ds = 2\Delta E\, dt/\hbar \tag{8}$$

is the infinitesimal distance between $\Pi(|\psi(t)\rangle)$ and $\Pi(|\psi(t+dt)\rangle)$. This proves that (3) is the distance along the evolution of the system in $\mathcal{P}$, as measured by the Fubini-Study metric, for both finite- and infinite-dimensional Hilbert spaces.

In the adiabatic limit considered by Berry[1] in which $|\psi(t)\rangle$ evolves as an eigenstate of $H(t)$, $\Delta E \to 0$ whereas $dt \to \infty$ so that ds is finite and nonzero. Hence this is a degenerate limit which is not useful in the study of physical manifestations of the Fubini-Study metric. Also, the above considerations show that even in the adiabatic limit, $\mathcal{P}$ is more useful and more geometrical than the parameter space used by Berry, which provides further support to the reformulation[2] of the geometric phase using $\mathcal{P}$.

As a simple application of this result, consider a spin-$\frac{1}{2}$ particle precessing in a homogeneous magnetic field. In this case $\mathcal{H} = \mathcal{C}^2$, $\mathcal{P} = P_1(\mathcal{C})$ is a sphere and the Fubini-Study metric defined above is the usual metric on this sphere corresponding to unit radius. At any instant of time, coordinate axes can be chosen so that the Hamiltonian $H = -\mu\sigma_z$ and the state is $|\psi\rangle = (\cos\frac{1}{2}\theta, \sin\frac{1}{2}\theta)$, where $\mu > 0$ and $\theta \in [0,\pi]$. Then, from (2), $\Delta E = \mu \sin\theta$. Also, from (1), $2\mu\, dt/\hbar = d\phi$ which is the infinitesimal angle by which the state is rotated about the instantaneous direction of the magnetic field in the infinitesimal time dt. Hence, $2\Delta E\, dt/\hbar = \sin\theta\, d\phi$, which verifies (8).

Equation (8) gives a new geometric meaning to the uncertainty in energy ΔE for an arbitrary quantum system: $ds/dt = 2\Delta E/\hbar$ is the magnitude of the *velocity* of the system in the projective Hilbert space. It follows that the evolution of the system in $\mathcal{P}$ completely determines ΔE; no other information from H is needed to determine ΔE. On the other hand, the distance s given by (3) is independent of even the rate of evolution and depends only on the unparametrized curve in $\mathcal{P}$ that is determined by the evolution.

Also, the time-energy uncertainty principle acquires a new geometric meaning as follows. To distinguish between two states in the history of the quantum system it is necessary for these states to be orthogonal, because they must be eigenstates of some Hermitian observable with different eigenvalues. Since the shortest possible distance between orthogonal states, which is along a geodesic, is π, the actual distance $s \geq \pi$, where s is given by (3) for the actual evolution between the two states. This may be rewritten as

$$\langle \Delta E \rangle \Delta t \geq \tfrac{1}{4} h\,, \tag{9}$$

where $\langle \Delta E \rangle$ is the time-averaged uncertainty in energy during the time interval Δt and h is Planck's constant. The inequality (9) is independent of our normalization convention for the Fubini-Study metric. It is more stringent than the usual time-energy uncertainty relation which has $\hbar/2$ on the right-hand side.[14] Equality in (9) holds if and only if the system moves along a geodesic in $\mathcal{P}$. In this case the *evolution* may be said to have minimum uncertainty analogous to how a Gaussian wave packet is said to have minimum position-momentum uncertainty at a given time. More generally we can define the efficiency of an evolution $\varepsilon = s_0/s$, where s_0 is the distance along the shortest geodesic joining the initial and final points of the evolution that are distinct points on $\mathcal{P}$. Then $\varepsilon \leq 1$, which contains (9) as a special case, but is valid more generally even when the system does not pass through orthogonal states.

As an application, consider a double-slit interference experiment in which we observe through which of the slits 1 and 2 the particle goes by letting it interact with a second system, which we take to be a spin-$\frac{1}{2}$ particle initially in the state $|\sigma_z = 1\rangle$. The particle interacts with the second system if and only if it goes through slit 2. The Hamiltonian of the interaction is $H = g(t)\sigma_x f(n)$, where $f(1) = 0$ and $f(2) = 1$ corresponding to the particle going through slit 1 or 2, respectively. The corresponding wave functions of the particle will be denoted by ψ_1 and ψ_2, respectively. Then the wave function of the combined system after the interaction is

$$\psi_1|\sigma_z = 1\rangle + \psi_2 \frac{1}{\sqrt{2}}\{\exp(i\phi_+)|\sigma_x = 1\rangle + \exp(i\phi_-)|\sigma_x = -1\rangle\}$$
$$= \frac{1}{\sqrt{2}}\{\psi_1 + \psi_2\exp(i\phi_+)\}|\sigma_x = 1\rangle + \frac{1}{\sqrt{2}}\{\psi_1 + \psi_2 \exp(i\phi_-)\}|\sigma_x = -1\rangle\,. \tag{10}$$

From the left-hand side of (10), the distance along a geodesic joining the initial and final spin states in the projective Hilbert space of the spin when it interacts with the particle, on using (6), is

$$\theta = |\phi_+ - \phi_-| \text{ or } 2\pi - |\phi_+ - \phi_-|\,. \tag{11}$$

From the right-hand side of (10), $|\phi_+ - \phi_-|$ is the phase difference between the particle state through slit 2 for the two possible spin eigenstates of H, which has a new geometric meaning given by (11). In particular when $\theta = \pi$, there is no interference between the two beams. Therefore, regardless of how weak the interaction between the two systems is, so long as the spin state undergoes a transition to an orthogonal state, the interference pattern is destroyed because of the minimum distance π between the two orthogonal states in the spin projective Hilbert space. Since the inequality (9) expresses the existence of this minimum distance, the loss of coherence in this experiment may also be regarded as due to this time-energy uncertainty principle.

As a further application, we show how a quantum-mechanical "clock" directly measures the Fubini-Study distance and that "time" is derived from this distance. A simple model of a clock is represented by the normalized state vector

$$|\psi(t)\rangle=(2J+1)^{-1/2}\sum_{n=-J}^{J}\exp\left(-\frac{in\eta t}{\hbar}\right)|n\rangle\,, \tag{12}$$

where $\{|n\rangle\}$ are fixed orthonormal states, η is a positive constant, and J is a large positive integer or half integer. This state vector passes through the sequence of orthonormal state vectors

$$|\psi_m\rangle=(2J+1)^{-1/2}\sum_{n=-J}^{J}\exp\left(-\frac{i2\pi nm}{2J+1}\right)|n\rangle\,, \quad m=-J,\ldots,J\,, \tag{13}$$

which may be regarded as the "pointer positions" of the clock.

A possible Hamiltonian for the evolution (12) satisfies $H|n\rangle=n\eta|n\rangle$, $n=-J,-J+1,\ldots,J$. Then from (2),

$$\Delta E=(\eta/\sqrt{3})(J^2+J)^{1/2}\,, \tag{14}$$

which, of course, is independent of t. Therefore, from (3),

$$s=(2\eta/\sqrt{3}\hbar)(J^2+J)^{1/2}t\,. \tag{15}$$

Hence, the Fubini-Study distance between two successive states (13), corresponding to the time interval $\Delta t=h/(2J+1)\eta$, is

$$\Delta s=\frac{4\pi(J^2+J)^{1/2}}{\sqrt{3}(2J+1)}\,, \tag{16}$$

which tends to the *universal value* $2\pi/\sqrt{3}$ as $J\to\infty$. This limiting distance is nonzero even though $\Delta t\to 0$ as $J\to\infty$. Also, it is greater than the shortest distance π between the states, as it should be because the clock is not moving along a geodesic. If it is desired to keep the Hamiltonian bounded below then J cannot become infinite. But J can be made arbitrarily large.

It is therefore clear that, for arbitrarily large J, the number of pointer positions through which the clock passes is proportional to s. Since time is measured by counting these pointer positions, the clock really measures s. The parameter t represents correlation between the Fubini-Study distances determined by different clocks. The above treatment clarifies the relationship between the parameter t which occurs in Schrödinger's equation and the time measured by a clock. Also, the greater ΔE the larger the change in s for a given change in t and hence the more accurate the reading of time by the clock. This is a particular application of the time-energy uncertainty principle.

Also, let ϕ be the variable conjugate to n. The inner product in the ϕ space is defined by

$$(f,g)=\frac{1}{2\pi}\int_0^{2\pi}f(\phi)g(\phi)d\phi\,.$$

Then, in ϕ space, the representations of $|n\rangle$ and $|\psi(t)\rangle$ are, respectively, $e^{in\phi}$ and

$$\psi(\phi,t)=(2J+1)^{-1/2}\sum_{n=-J}^{J}\exp(inx) =(2J+1)^{-1/2}\frac{\sin\{(J+\frac{1}{2})x\}}{\sin(\frac{1}{2}x)}\,, \tag{17}$$

where $x=(\phi-\eta t/\hbar)$. Hence, for large J, $\psi(\phi,t)$ is sharply peaked around $\phi=\eta t/\hbar$. Indeed, $(2J+1)^{1/2}\times\psi(\phi,t)$ tends to the Dirac delta function $\delta(\phi-\eta t/\hbar)$ as $J\to\infty$. The center of $\psi(\phi,t)$ moves around ϕ space with constant angular speed $\omega=\eta/\hbar$ with its shape fixed. Therefore, the clock is well behaved at all times as $J\to\infty$. From (15), ω is proportional to ds/dt. Hence, the measurement of s by the clock is in effect also a measurement of angular distance traveled in ϕ space, corresponding to the displacement of its pointer position.

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[a]Also at the Max-Planck-Institute for Physics and Astrophysics, Fohringer Ring 6, D-8000 Munich 40, Federal Republic of Germany. On leave from the Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208.

[b]Also at the Department of Physics, Tel Aviv University, Ramat Aviv, Israel.

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