Foundations of Physics, Vol. 21, No. 11, 1991

A Geometric Approach to Quantum Mechanics[1]

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Received November 26, 1990; revised May 20, 1991

It is argued that quantum mechanics is fundamentally a geometric theory. This is illustrated by means of the connection and symplectic structures associated with the projective Hilbert space, using which the geometric phase can be understood. A prescription is given for obtaining the geometric phase from the motion of a time dependent invariant along a closed curve in a parameter space, which may be finite dimensional even for nonadiabatic cyclic evolutions in an infinite dimensional Hilbert space. Using the natural metric on the projective space, we reformulate Schrödinger's equation for an isolated system. This metric is generalized to the space of all density matrices, and a physical meaning is proposed.

1. INTRODUCTION

This paper is based on the view that the world is ultimately geometrical. We know that in some fields of physics, especially general relativity, geometric ideas have been very useful. But the deepest physical theory we have today is quantum theory where geometric ideas are not readily apparent. Some quantum theorists have therefore argued that we must regard gravity quantum mechanically as a spin-2 field and that the beautiful geometry in general relativity is really not needed. I wish to reverse this argument in this paper. I shall argue that there are interesting geometric structures in quantum theory also, and that perhaps we should look at

[1] Based on the talk delivered by the author at the Conference on Fundamental Aspects of Quantum Theory to celebrate 30 years of the Aharonov–Bohm effect, Columbia, South Carolina, December 14–16, 1989, published in *Quantum Coherence*, J. S. Anandan, ed. (World Scientific, 1990).

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825/21 11-1

0015-9018/91/1100-1265$06.50/0

quantum theory as a geometric theory, like special relativity formulated using Minkowski space-time.

The important role played by geometric ideas in quantum theory may be illustrated by examples beginning with the creation of quantum theory itself. As is well known, an important role was played in this creation by Hamilton's reformulation of classical mechanics, which inspired De Broglie and Schrödinger to discover wave-particle duality and quantum mechanics. What was Hamilton's motivation for doing this even though Newton's original formulation of classical mechanics was very intuitive and physical?

The answer is that Hamilton originally studied geometric optics in which the central question is the following: Given a set of rays entering an optical system, what is the set of outgoing rays? Each set of rays may be parametrized by the coordinates x, y of the point at which a typical ray intersects a fixed plane perpendicular to the optical axis and by p_x, p_y that are the corresponding direction cosines of the ray at this point multiplied by the refractive index. (In the wave description, p_x and p_y are proportional to the components of the wave vector along the x and y axes.) In modern terms, he found the transformation between the two sets of rays to be symplectic,[1] i.e., it preserves the symplectic structure in the space $\{(x, y, p_x, p_y)\}$. A few years later it occurred to Hamilton that if the optical axis is taken to be the time axis, then classical mechanics in two spatial dimensions can be reformulated using the same symplectic geometry, which is easily extended to any number of dimensions of the configuration space. Using this symplectic structure, the Poisson bracket between any two observables is formed. And the well-known Dirac prescription to replace Poisson brackets by commutators gives quantum mechanics.

The second example that I wish to give is the Aharonov–Bohm (AB) effect.[2] The most important lesson to me from this effect is that the classical electromagnetic field should be described geometrically as a connection, which is discussed elsewhere.[3] Then the AB phase factor is the holonomy transformation when the value of the wave function at an event in the interference region is parallel transported with respect to the electromagnetic connection around a closed curve, which passes through the interfering beams.

Whereas the above two examples have been studied in great detail over the years, the third example which I wish to mention is of recent origin. This is the geometric phase. Suppose a quantum system undergoes cyclic evolution, by which I mean that its state vector $|\psi(t)\rangle$ obeys Schrödinger evolution in the interval $[0, \tau]$ such that $|\psi(\tau)\rangle = e^{i\phi}|\psi(0)\rangle$. It was shown[4,5] that there is a part β of the total phase ϕ acquired which is geometric in the sense that it depends only on the motion of the system given by a closed curve C in the set of rays of the Hilbert space $\mathscr{H}$, which

is called the projective Hilbert space $\mathscr{P}$, and is independent of the particular Hamiltonian used to obtain this motion.

This β can be understood in two ways. First, $e^{i\beta}$ is the holonomy transformation for parallel transporting around C in $\mathscr{P}$, or around a closed curve γ in a parameter space defined in Section 2, with respect to the natural connection given by the inner product in $\mathscr{H}$.[5,6] From this viewpoint, β is like the AB phase. Alternatively, β is the "area" of any surface spanned by C with respect to the natural symplectic structure in $\mathscr{P}$ determined by this inner product.[3,7] Interestingly, this symplectic structure when restricted to the submanifold of Gaussian wave packets with constant width, which may be identified with the classical phase space, is the symplectic structure found by Hamilton in the latter space.[3] Therefore, what Hamilton found, which made his reformulation of Newtonian mechanics so powerful, was a "shadow" of a geometric structure in quantum mechanics. Similar to how Hamilton's geometric reformulation of classical mechanics paved the way for quantum mechanics, perhaps, a geometric reformulation of quantum mechanics may lead to a new physical theory which we need today for a proper description of gravity, consistent with quantum phenomena.

2. GEOMETRIC PHASE AND CONNECTION

The geometric phase is a consequence of just the inner product and is independent of the particular equation of motion which is first order in time.[8] But for simplicity, we shall now obtain it as a consequence of the Schrödinger evolution

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

where H is the Hamiltonian and $\langle\psi(t)|\psi(t)\rangle = 1$. Given the cyclic evolution described above, choose $|\tilde{\psi}(t)\rangle$ such that $|\psi(t)\rangle = \xi(t) |\tilde{\psi}(t)\rangle$, where the function[9] $\xi(t)$ has complex values with unit modulus, and $|\tilde{\psi}(\tau)\rangle = |\tilde{\psi}(0)\rangle$. Then (1) implies

$$i\hbar \left(\frac{d}{dt} + \langle\tilde{\psi}(t)| \frac{d}{dt} |\tilde{\psi}(t)\rangle \right) \xi(t) = \langle\psi(t)| H |\psi(t)\rangle \xi(t) \tag{2}$$

The left-hand side of (2) does not depend on the Hamiltonian and suggests the introduction of the covariant derivative:

$$\frac{D}{dt} \equiv \frac{d}{dt} + \langle\tilde{\psi}(t)| \frac{d}{dt} |\tilde{\psi}(t)\rangle \equiv \mathbf{v} \cdot \nabla$$

where $\nabla = d + \langle\tilde{\psi}|\, d\,|\tilde{\psi}\rangle$, d being the exterior differential operator on $\mathscr{P}$, and $\mathbf{v}$ is the "velocity" in $\mathscr{P}$, i.e., $\mathbf{v}$ is the tangent vector to the curve C in $\mathscr{P}$ parametrized by t, representing the evolution. Here $|\tilde{\psi}\rangle$ is a "section" defined in some neighborhood U of C and $\langle\tilde{\psi}|\, d\,|\tilde{\psi}\rangle$ represents the "connection form" with respect to this section. $\langle\tilde{\psi}|\, d\,|\tilde{\psi}\rangle$ is analogous to ieA, where A is the electromagnetic vector potential, which is a connection form over space-time. The normalization $\langle\tilde{\psi}|\tilde{\psi}\rangle = 1$ implies that $\langle\tilde{\psi}|\, d\,|\tilde{\psi}\rangle$ is pure imaginary. If a different section $|\tilde{\psi}'\rangle = e^{ig}\,|\tilde{\psi}\rangle$ is chosen, where g is a real differentiable function on U, then ξ transforms to $e^{-ig}\xi$ and $\langle\tilde{\psi}|\, d\,|\tilde{\psi}\rangle$ transforms to $\langle\tilde{\psi}|\, d\,|\tilde{\psi}\rangle + i\, dg$, which is analogous to the electromagnetic gauge transformation. Clearly, (2) is covariant under this "local gauge" transformation.

Equation (2) can be integrated immediately to yield

$$\xi(\tau) = \exp\left\{-\oint_C \langle\tilde{\psi}|\, d\,|\tilde{\psi}\rangle - \frac{i}{\hbar}\int_0^\tau \langle\psi|\, H(t')\,|\psi\rangle\, dt'\right\}\xi(0) \tag{3}$$

The real phase

$$\beta \equiv i\oint_C \langle\tilde{\psi}\,|\,d\tilde{\psi}\rangle = i\int_\Sigma \langle d\tilde{\psi}|\wedge|d\tilde{\psi}\rangle \tag{4}$$

where Σ is a surface spanned by C and $|d\tilde{\psi}\rangle = d\,|\tilde{\psi}\rangle$, is called the geometric phase, because $e^{i\beta}$ is the holonomy transformation associated with C with respect to the connection mentioned above, i.e., if we parallel transport a function η around according to the rule $D\eta/dt = 0$, then it acquires the phase factor $e^{i\beta}$. Also, $e^{i\beta}$ is invariant under a change of section similar to how the Aharonov–Bohm[2] phase factor $\exp[(ie/\hbar)\oint A_\mu\, dx^\mu]$ is invariant under gauge transformations.

It may appear at first sight that it would be necessary to solve the full quantum mechanical problem in order to determine the path C and thereby predict $e^{i\beta}$. But this is not the case. I shall show now that for an arbitrary $H(t)$ it is possible to determine $e^{i\beta}$ by solving the classical problem and an eigenvector problem for a set of invariants defined below. Suppose we have a class of Hamiltonians of the form $H(R) = \hbar R^\alpha J_\alpha$ where R^α are real variables and iJ_α generate a subgroup of the unitary group G determined by the Lie algebra relations

$$[J_\alpha, J_\beta] = iC_{\alpha\beta}{}^\gamma J_\gamma \tag{5}$$

Therefore, $C_{\alpha\beta\gamma}$ is totally antisymmetric, with the index being lowered using the metric $\delta_{\alpha\beta}$. Let $I(S) = S^\alpha J_\alpha$, where S^α are a set of parameters. Each

$S=(S^1, S^2,...)$ is a point in a parameter space $\mathscr{S}$. Now, let $|n(S)\rangle$ be a complete set of orthonormal eigenstates of a Hermitian operator $I(S)$:

$$I(S)\,|n(S)\rangle = I_n(S)\,|n(S)\rangle \tag{6}$$

Suppose $|\psi_n(t)\rangle$ evolves according to Schrödinger's equation, i.e., $|\psi_n(t)\rangle \equiv U(t)\,|\psi_n(0)\rangle$, where $U(t)$ is the time evolution operator:

$$U(t) = T\exp\left\{-\frac{i}{\hbar}\int_0^t H(t')\,dt'\right\}$$

where T denotes time ordering. Let $S(t)$ be a curve in $\mathscr{S}$ in the interval $[0, \tau]$, such that each $|\psi_n(t)\rangle$ is an eigenstate of $I(S(t))$ with a constant eigenvalue I_n. This curve is not unique. But on requiring that $I(S(t)) = U(t)\,I(S(0))\,U^\dagger(t) \equiv S^\alpha(t)\,J_\alpha$, $S(t)$ is unique for a given $S(0)$. Then

$$\frac{\partial I}{\partial t} - \frac{i}{\hbar}[I, H] = 0 \tag{7}$$

i.e., $I(S(t))$ is an explicitly time-dependent Schrödinger observable which is an invariant of the motion.[10] Conversely, if I satisfies (7), then by reversing the steps, it follows that if $|\psi(t)\rangle$ was initially an eigenstate of $I(S(t))$ then it continues to be in an eigenstate with the same eigenvalue.

Suppose that the curve is closed, i.e., $S(\tau) = S(0)$, and denote the unparametrized closed curve by γ. In general, $|\psi_n(0)\rangle$ and $|\psi_n(\tau)\rangle$ need not belong to the same eigensubspace of $I(S(0)) = I(S(\tau))$. For example, if I has an infinite spectrum, then it is possible for the nth state to go into the $(n+1)$th state during the cyclic evolution of I. But this is very unusual and we shall suppose here the usual case of them belonging to the same eigensubspace. I assume for the present that $I(S)$ is nondegenerate for every S. Then $|\psi_n(\tau)\rangle = e^{i\phi_n}\,|\psi_n(0)\rangle$ for some ϕ_n. Then, as shown by (3), ϕ_n is the sum of the dynamical phase and the geometric phase β_n.[11] $|\psi_n(t)\rangle$ is proportional to $|n(S(t))\rangle$, and therefore $I(S(t)) = \sum_n I_n\,|\psi_n(t)\rangle\langle\psi_n(t)|$. Also, β_n may be obtained from (4) by replacing $|\tilde{\psi}\rangle$ by $|n(S)\rangle$:

$$\beta_n \equiv i\oint_\gamma \langle n(S)\,|\,dn(S)\rangle = i\int_\sigma \langle dn(S)|\wedge|dn(S)\rangle \tag{8}$$

where σ is a surface spanned by γ and d is now the exterior differential operator on *parameter space*. Geometrically, $e^{i\beta_n}$ may be regarded as the holonomy transformation with respect to a connection in a line bundle

over the space $\mathscr{S}$, whose fiber over $S \in \mathscr{S}$ is the eigensubspace of $I(S)$ with eigenvalue $I_n(S)$, and the pullback of the connection form by a local section $|n(S)\rangle$ is $\langle n(S)|\, dn(S)\rangle$.

To determine γ, we obtain from (5) and (7),

$$\frac{dS^\alpha}{dt} = -C_{\beta\gamma}{}^{\alpha} S^\beta R^\gamma \tag{9}$$

It follows that $S_\alpha S^\alpha$ is a constant of motion. Therefore, for inessential economy, we may restrict our parameter space to the sphere $\mathscr{S}'$ in $\mathscr{S}$ defined by the condition $S_\alpha S^\alpha = 1$. The line bundle and the connection described above may accordingly be restricted to be over $\mathscr{S}'$. Equation (9) can be given the following classical interpretation: Let $H^c \equiv R^\alpha T_\alpha$ be the classical Hamiltonian obtained by replacing $\hbar J_\alpha$ in H by a set of classical observables T_α which obey the Poisson bracket relations

$$\{T_\alpha, T_\beta\} = C_{\alpha\beta}{}^{\gamma} T_\gamma \tag{10}$$

The T_α may be regarded as the classical limit of the quantum observables $\hbar J_\alpha$. Also, replace I by the classical observable $I^c(t) = S^\alpha(t)\, T_\alpha$ which is required to be an invariant of the evolution under H^c:

$$\frac{\partial I^c}{\partial t} + \{I^c, H^c\} = 0 \tag{11}$$

On using (10), (11) yields (9). Hence (9) may be regarded as the classical equation of motion for S^α. By solving it, the curve γ and hence the geometric phase (8) can be obtained.

From (6),

$$(I_n(S) - I_m(S))\langle m(S)|\, dn(S)\rangle = \langle m(S)|\, dI(S)\, |n(S)\rangle, \qquad m \neq n \tag{12}$$

Therefore, Eq. (8) may be rewritten, after inserting a complete set of states and using (12), as

$$\beta_n = i \int_\sigma \sum_{m \neq n} \frac{\langle n|\, dI\, |m\rangle \wedge \langle m|\, dI\, |n\rangle}{(I_n - I_m)^2} \tag{13}$$

There is no contribution $m = n$ in the summation over m in (13), because $\langle n(S)|\, dn(S)\rangle$ is pure imaginary, due to the normalization of $|n(S)\rangle$, and therefore its wedge product with its complex conjugate vanishes. The prescription (13) has the advantage that $|n(S)\rangle$ need not be chosen differentiably or even continuously over the parameter space, unlike the prescription (8). This is similar to the prescription given by Berry[4] to

evaluate the geometric phase in the adiabatic limit using the parameter space $\mathscr{R}$ consisting of possible values of R^α with the Hamiltonian $H(R)$ playing the role of $I(S)$. In this limit, the evolving state may also be taken as an approximate eigenstate of $H(R)$. Then S^α may taken to be parallel to R^α. But we prefer, even in this limit, to regard $\mathscr{S}$ as the parameter space for the evaluation of the geometric phase instead of $\mathscr{R}$. Because, even when the curve in $\mathscr{R}$ defined by $H(R(t))$ is not closed, the evolution may still be cyclic because the corresponding curve $S(t)$ in $\mathscr{S}$ satisfying (9) is closed. Also, the present approach gives the freedom to take more general states which are not eigenstates of H, even in the adiabatic limit. We can always construct an explicitly time-dependent invariant operator $I(S(t))$ whose eigenstate $|\psi(t)\rangle$ is, and the geometric phase for a cyclic evolution may be obtained from the above prescription.

As an example, consider the precession of an arbitrary spin in an arbitrary magnetic field $\mathbf{B}(t)$.[12] Then the Hamiltonian may be written as $H = -\eta\hbar\mathbf{B}\cdot\mathbf{J}$, where iJ_α generate $SU(2)$. Therefore, here $R^\alpha = -\eta B^\alpha$ and (9) is

$$\frac{d\mathbf{S}}{dt} = \eta\mathbf{S}\times\mathbf{B} \tag{14}$$

Here, the parameters S^α may be given a classical meaning as the components of a spin vector; then $\mu = \eta\mathbf{S}$ is the magnetic moment. Equation (14) is the classical equation of motion for spin. By solving it, we obtain a curve in $\mathscr{S}$ which is unique for given initial $\mathbf{S}$. The curve lies in $\mathscr{S}'$ which is the sphere in $\mathscr{S}$ with its center at the origin and its radius equal to the magnitude of the initial vector $\mathbf{S}$. When this curve γ is closed, the evolution is cyclic. The geometric phase is obtained now from the holonomy transformation associated with γ with respect to the connection defined over $\mathscr{S}'$, or it may be evaluated using (13). It can be shown[11] that $\beta_n = j_n\alpha$, where α is the solid angle subtended by γ at the origin.

Another example is a finite-dimensional Hilbert space $\mathscr{H}$ of dimension N with H being an arbitrary Hermitian operator in $\mathscr{H}$. A Cartan subalgebra of $U(N)$, which acts on $\mathscr{H}$, is generated by matrices J_k, $k = 1,..., N$, where the only nonzero element of J_k is the kth diagonal element which is equal to 1. Let $I_0 = \sum_{k=1}^N \lambda^k J_k$, whose eigenvalues λ^k are chosen to be distinct. Given the orthonormal basis of initial states $\{|\psi_n(0)\rangle\}$, there is a unitary transformation V which maps this basis onto the normalized eigenstates of I_0. Then $I(S) \equiv V^\dagger I_0 V \equiv S^\alpha J_\alpha$ has $\{|\psi_n(0)\rangle\}$ as eigenstates with distinct eigenvalues λ^k, where $\{J_\alpha\}$ is a basis for the Lie algebra of $U(N)$, i.e., $\{J_\alpha\}$ generates the set of all $N\times N$ Hermitian matrices. The geometric phase for each $|\psi_n\rangle$ can be obtained from the holonomy of the connection over $\mathscr{S}$ as described above.

We therefore have now the following general prescription for obtaining the geometric phase: Given an arbitrary cyclic quantum evolution of a state, associate with it a motion of an explicitly time dependent *invariant*. This motion is obtained as a closed curve in the space $\mathscr{S}$ of possible values of the corresponding classical quantity, by solving the *classical* equations of motion. There is a natural connection over $\mathscr{S}$ for parallel transporting eigenstates of this invariant. The geometric phase factor is the same as the holonomy transformation associated with this curve with respect to this connection. There are an infinite number of Hamiltonians which give rise to a given *motion* of the invariant, defined by an unparametrized curve γ in $\mathscr{S}$. An adiabatic Hamiltonian, for example, is one way of achieving this motion. But the geometric phases for the eigenstates of I are a property of this motion and independent of the particular choice of the Hamiltonian.

More generally, if $I(S)$ is degenerate, then the cyclic evolution of $I(S)$ may be associated with the cyclic evolution of an eigensubspace whose dimension m may be greater than one. The geometric phase factor is then generalized to an element of $SU(m)$, which is described elsewhere.[13]

3. SYMPLECTIC STRUCTURE

Another geometric meaning can be given to β as the symplectic area enclosed by C determined by the natural symplectic structure on $\mathscr{P}$ inherited from the symplectic structure in $\mathscr{H}$ due to the inner product.[3] More specifically, define the canonical coordinates and momenta $Q^j = \psi_j$ and $P_j = i\hbar\bar{\psi}_j$, where ψ_j are the components of $|\psi\rangle$ in an arbitrary orthonormal basis and the overbar denotes complex conjugation. Then (4) may be rewritten as

$$\beta = \frac{1}{\hbar}\oint_C P_j\, dQ^j = \frac{1}{\hbar}\int_\Sigma dP_j \wedge dQ^j \tag{15}$$

Here $\hbar$ is used in the definition of P_j only in order that the integral in (15) has the dimension of action.

On the other hand, the action for the Schrödinger field is

$$S = \frac{1}{2}\int dt \left(i\hbar \left\langle \psi \middle| \frac{d}{dt}\psi \right\rangle - i\hbar \left\langle \frac{d}{dt}\psi \middle| \psi \right\rangle - 2\langle \psi |\, H\, | \psi \rangle \right) = \int d^4x\, \mathscr{L} \tag{16}$$

Then the momentum conjugate to the canonical coordinate Q^j is

$$\frac{\partial \mathscr{L}}{\partial \dot{Q}^j} = i\hbar\bar{\psi}_j = P_j$$

Thus we obtain, using dynamical considerations, the same pairs of canonically conjugate coordinate and momentum obtained earlier by purely geometric considerations; i.e., the symplectic structure given by the Lagrangian density $\mathscr{L}$ is the same as the symplectic structure given by (15). In general, this is true whenever the equation of motion is first order in the time derivative. Therefore, in some sense, *the geometry is prior to the dynamics* here. Also, the procedure of second quantizing the Schrödinger field by imposing canonical commutation relations between P_j and Q_j, regarded as operators, uses the above symplectic structure determined by the inner product on $\mathscr{H}$.

We can go in the opposite direction of taking the classical limit of the first quantized theory. This may be done by using isotropic Gaussian states centered around a classical phase space point $(\mathbf{q}, \mathbf{p})$ with a constant width Δq in coordinate space:

$$\tilde{\psi}_{\mathbf{q},\mathbf{p}}(\mathbf{x}) = \{2\pi(\Delta q)^2\}^{-1/4} \exp\left\{-\frac{(\mathbf{x}-\mathbf{q})^2}{(2\Delta q)^2} + \frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{x}-\mathbf{q})\right\} \tag{17}$$

In the classical limit, the quantum system has a large enough mass for the spreading of the wave packet to be negligible during the time interval of interest. Then its state may be assumed to remain in the form (17), up to phase, with $(\mathbf{q}, \mathbf{p})$ changing with time, to a very good approximation. Therefore, the submanifold $\mathscr{C}$ of $\mathscr{P}$ consisting of the states (17), for a fixed Δq, may be identified with the classical phase space $\{(\mathbf{q}, \mathbf{p})\}$.

Consider a cyclic motion $(\mathbf{q}(t), \mathbf{p}(t))$ that is a closed curve C in $\mathscr{C}$. Then

$$i\langle\tilde{\psi}_{\mathbf{q}(t),\,\mathbf{p}(t)}|\frac{d}{dt}|\tilde{\psi}_{\mathbf{q}(t),\,\mathbf{p}(t)}\rangle = \frac{1}{\hbar}\mathbf{p}\cdot\frac{d\mathbf{q}}{dt} \tag{18}$$

Hence the geometric phase for this motion, using (4) and Stoke's theorem, is[3,7]

$$\beta = \frac{1}{\hbar}\int_S d\mathbf{p}\wedge\cdot d\mathbf{q} \tag{19}$$

where S is a surface in $\mathscr{C}$ spanned by C. On comparing (19) with (15), it is clear that $(1/\hbar)\,d\mathbf{p}\wedge\cdot d\mathbf{q}$ is the restriction to $\mathscr{C}$ of the symplectic form in $\mathscr{P}$, defined above. Hence, β may be regarded, in this classical limit, as the symplectic "area" in the classical phase space and is therefore a canonical invariant.

The above treatment of the geometric phase therefore suggests why Hamilton's reformulation of classical mechanics should be much closer to

quantum mechanics than Newton's original formulation: The symplectic structure used by Hamilton is close to the inner product in $\mathscr{H}$, whereas there is no such geometric structure in Newton's formulation. Hamilton's equations of motion determine a family of trajectories in the classical phase space $\mathscr{C}$ for a given Hamiltonian, which generates a 1-parameter family of transformations along these trajectories which preserve the symplectic structure. When the theory is quantized, the classical states may be represented approximately by Gaussian wave packets; but it now becomes possible to take superpositions of them to form the Hilbert space $\mathscr{H}$. These wave packets can spread and therefore Hamiltonian classical mechanics should be regarded as the geometric optics limit of quantum mechanics. But in $\mathscr{H}$, there is a symplectic 2-form $\Omega = (1/\hbar)\, dP_j \wedge dQ^j$, which gives $\Omega(\psi, \phi) = -2\,\mathrm{Im}\langle\psi|\phi\rangle$ for any two tangent vectors ψ, ϕ of $\mathscr{H}$. Since Schrödinger's equation preserves the inner product, it must preserve Ω. As seen above, the classical limit of Ω is $\omega = dp_j \wedge dq^j$, which determines the symplectic structure in $\mathscr{C}$. Therefore we expect ω to be preserved in the classical limit, which is satisfied by Hamilton's equations.

4. METRIC

The inner product also gives the following distance function on $\mathscr{P}$: The distance s between any two points p and p' in $\mathscr{P}$ is defined by

$$s(p, p')^2 = 4(1 - |\langle\psi|\psi'\rangle|^2)$$

where $|\psi\rangle$ and $|\psi'\rangle$ are two normalized states contained in p and p'. Clearly, $s(p, p') \geqslant 0$ with equality holding if and only if $p = p'$. Also $s(p, p') = s(p', p)$. The triangle inequality

$$s(p, p') + s(p', p'') \geqslant s(p, p'')$$

can be shown to be valid for any p, p' and p'' in $\mathscr{P}$. Hence s is a metric on $\mathscr{P}$. Physically, $s(p, p')$ represents the probability of a system initially in state $|\psi\rangle$ remaining in the same state after a measurement is made to see if it is in state $|\psi'\rangle$. To gain further geometric insight into this metric, consider the projective space $P_1(\mathscr{C})$ corresponding to the subspace spanned by $|\psi\rangle$ and $|\psi'\rangle$. The above metric when restricted to $P_1(\mathscr{C})$ enables it to be regarded as a 2-sphere with unit radius embedded in a real three-dimensional Euclidean space, and $s(p, p')$ is then the straightline distance between p and p' on this sphere.

Suppose that p and p' are separated by an infinitesimal distance ds in $\mathscr{P}$:

$$ds^2 = 4(1 - |\langle\psi|\psi'\rangle|^2) \tag{20}$$

We may alternatively define a Riemannian metric on $\mathscr{P}$ by (20). This is a Kahler metric, called the Fubini–Study metric.[15] For the purpose of a result in Section 5, I now use fiber bundles to give in a natural manner the latter metric as well as the connection and the symplectic structure discussed in Sections 2 and 3, respectively. Alternative definitions of this metric are also given in (24) and (31).

Suppose $\mathscr{H}$ has dimension $N+1$, where N is a nonnegative integer. The unitary group $U(N+1)$ acting on $\mathscr{H}=\mathscr{C}^{N+1}$ can be identified with the set $\mathscr{B}$ of orthonormal bases of $\mathscr{H}$ because each element of $\mathscr{B}$ can be obtained from a fixed element of $\mathscr{B}$ 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 $\mathscr{B}$, which is the same as $U(N+1)/U(N)$, may be identified with the set of unit vectors of $\mathscr{H}$ 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 $\mathscr{P}=P_N(\mathscr{C})$, 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 $\mathscr{P}$ 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 $\mathscr{P}$ 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 an $(N+1)$-dimensional Hermitian matrix. Define the metric h in $\mathscr{B}$ by the condition $h(X, Y)=2\,\mathrm{tr}(XY)$, where X and Y are tangent vectors at any point in $\mathscr{B}=U(N+1)$. 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 $\mathscr{P}$ 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 connection over the parameter space $\mathscr{S}$ or $\mathscr{S}'$ defined in Section 3 may also be understood as follows. Let α be the map from $\mathscr{S}$ into $\mathscr{P}$ which takes each $S\in\mathscr{S}$ into the one-dimensional eigensubspace of $I(S)$ corresponding to the eigenvalue $I_n(S)$. The pullback of S_N with the above connection by the map α is a $U(1)$ principal fiber bundle over $\mathscr{S}$ with a connection. The closed curve γ is mapped by α into the closed curve C. The geometric phase factor[5] $e^{i\beta}$ is obtained as the holonomy transformation,

i.e., parallel transport around C in $\mathscr{P}$ with respect to the connection in S_N or around γ in $\mathscr{S}$ with respect to the last mentioned connection.

Suppose that $|\psi\rangle$ and $|\psi'\rangle$ are such that $\Pi(|\psi\rangle)$ and $\Pi(|\psi'\rangle)$ are separated by an infinitesimal distance ds in $\mathscr{P}$. Then, it can be shown that[14] ds^2 is given by (20). To obtain the metric coefficients, consider a smooth curve $|\psi(t)\rangle$ in $\mathscr{B}$ such that $|\psi(t)\rangle$ and $|\psi(t+dt)\rangle$ project to $\Pi(|\psi\rangle)$ and $\Pi(|\psi'\rangle)$, respectively. Now,

$$\langle\psi(t)|\psi(t+dt)\rangle = 1 + dt\left\langle\psi\left|\frac{d}{dt}\psi\right.\right\rangle + \frac{1}{2}dt^2\left\langle\psi\left|\frac{d^2}{dt^2}\psi\right.\right\rangle + O(dt^3) \quad (21)$$

Also, differentiating $\langle\psi(t)|\psi(t)\rangle = 1$ twice, we have

$$\left\langle\psi\left|\frac{d}{dt}\psi\right.\right\rangle + \left\langle\frac{d}{dt}\psi\middle|\psi\right\rangle = 0$$

and (22)

$$\left\langle\psi\left|\frac{d^2}{dt^2}\psi\right.\right\rangle + \left\langle\frac{d^2}{dt^2}\psi\middle|\psi\right\rangle + 2\left\langle\frac{d}{dt}\psi\middle|\frac{d}{dt}\psi\right\rangle = 0$$

From (20), (21), and (22),

$$\left(\frac{ds}{dt}\right)^2 = 4\left\langle\frac{d}{dt}\psi\middle|\frac{d}{dt}\psi\right\rangle - 4\left\langle\frac{d}{dt}\psi\middle|\psi\right\rangle\left\langle\psi\middle|\frac{d}{dt}\psi\right\rangle \quad (23)$$

Therefore, in terms of an arbitrary section $|\tilde{\psi}\rangle$, the metric can be written as

$$ds^2 = 4(\langle d\tilde{\psi}\,|\,d\tilde{\psi}\rangle - \langle d\tilde{\psi}\,|\,\tilde{\psi}\rangle\langle\tilde{\psi}\,|\,d\tilde{\psi}\rangle) = 2g_{\bar{\mu}\nu}\,d\bar{z}^{\mu}\,dz^{\nu} \quad (24)$$

where z^{μ} are complex coordinates in $\mathscr{P}$ and the metric coefficients

$$g_{\bar{\mu}\nu} = 2\left(\left\langle\frac{\partial}{\partial z^{\mu}}\tilde{\psi}\middle|\frac{\partial}{\partial z^{\nu}}\tilde{\psi}\right\rangle - \left\langle\frac{\partial}{\partial z^{\mu}}\tilde{\psi}\middle|\tilde{\psi}\right\rangle\left\langle\tilde{\psi}\middle|\frac{\partial}{\partial z^{\nu}}\tilde{\psi}\right\rangle\right) \quad (25)$$

constitute a Hermitian matrix.[16] It can be verified that (24) is invariant under change of section $|\tilde{\psi}\rangle \to |\tilde{\psi}'\rangle = e^{ig}|\tilde{\psi}\rangle$. It may be regarded as an alternative definition of the Fubini–Study metric which is valid also for an infinite-dimensional $\mathscr{H}$. A unitary or anti-unitary transformation leaves the absolute value of the inner product invariant and is therefore an isometry in $\mathscr{P}$.

Equation (23) and hence the expression (24) for the metric may also be obtained in another way. The horizontal component of the tangent vector $(d/dt)\,|\psi\rangle$ is $(d/dt)\,|\psi\rangle - \langle\psi|\,d/dt\,|\psi\rangle\,|\psi\rangle$. Since the Fubini–Study metric on $\mathscr{P}$ is obtained by requiring that Π be a Riemannian submersion, twice the norm of the latter vector with respect to the inner product in $\mathscr{H}$ is ds/dt. This gives (23).

Also, the restriction of this metric to the submanifold $\mathscr{C}$ of $\mathscr{P}$ consisting of Gaussian wave packets of constant width Δq, defined in Section 3, yields an Euclidean metric[7] on $\mathscr{C}$, identified with the classical phase space, which can be written as

$$ds^2 = \lambda\, d\mathbf{q}^2 + \lambda^{-1}\, d\mathbf{p}^2$$

where $\lambda = \Delta p/\Delta q = 2\,\Delta p^2/\hbar = \hbar/2\,\Delta q^2$, Δp being the uncertainty in momentum. If $g^{\alpha\beta}$ are the coefficients of the inverse of this metric and $\omega_{\alpha\beta}$ the coefficients of the usual symplectic 2-form in the classical phase space $\mathscr{C}$, then it is easily verified that

$$\omega_{\alpha\beta}\, g^{\beta\gamma} = J^{\gamma}{}_{\alpha}$$

is a complex structure on $\mathscr{C}$, i.e., J satisfies

$$J^{\alpha}{}_{\beta} J^{\beta}{}_{\gamma} = -\delta^{\alpha}{}_{\gamma}$$

5. GEOMETRY OF QUANTUM EVOLUTION

I shall now give a geometric description of quantum evolution, which need not be cyclic, by means of the Fubini–Study metric on $\mathscr{P}$ described in Section 4. Suppose $|\psi(t)\rangle$ undergoes Schrödinger evolution. Then from (1) and (23), the speed of the quantum system in $\mathscr{P}$ is[14,17]

$$\frac{ds}{dt} = 2\,\frac{\Delta E}{\hbar} \tag{26}$$

where ΔE is the uncertainty in energy: $\Delta E^2 = \langle\psi(t)|\, H^2\, |\psi(t)\rangle - \langle\psi(t)|\, H\, |\psi(t)\rangle^2$. Hence the Fubini–Study distance s traveled during the time interval (t_1, t_2) is

$$s = 2\int_{t_1}^{t_2} \frac{\Delta E(t)}{\hbar}\, dt \tag{26'}$$

Suppose s_0 is the distance along the shortest geodesic joining $\Pi(|\psi(t_1)\rangle)$ and $\Pi(|\psi(t_2)\rangle)$, which I shall call the displacement between the two states. Then,

$$s \geqslant s_0 \tag{27}$$

But the above geodesic is also a geodesic on the sphere $P_1(C)$, the projective space of the subspace spanned by $|\psi(t_1)\rangle$ and $|\psi(t_2)\rangle$, which is an arc of a great circle.[5,14] Therefore (27) is the same as

$$\int_{t_1}^{t_2} \frac{\Delta E(t)}{\hbar}\, dt \geqslant \cos^{-1}(|\langle\psi(t_1)|\psi(t_2)\rangle|) \tag{27'}$$

Now, define the "uncertainty of time" $\Delta t = (\pi/s_0)(t_1 - t_2)$, assuming $s_0 \neq 0$. This amounts to rescaling the actual time interval by the ratio of the displacement π between two orthogonal states to the displacement s_0 during

the actual evolution. Then, in the special case where the initial and final states are orthogonal, $\Delta t = t_1 - t_2$. Conversely, the latter condition may be used to constrain the rescaling factor. Then, (27) reads

$$\langle \Delta E \rangle \, \Delta t \geq \frac{h}{4} \tag{28}$$

where h is Planck's constant and $\langle \Delta E \rangle$ is the time-averaged uncertainty of energy in the interval (t_1, t_2). This is in the form of a time–energy uncertainty relation, which was previously obtained for the special case where the initial and final states are orthogonal.[14] But (28) is valid more generally when the system does not pass through orthogonal states. The usual problem in deriving the time–energy uncertainty relation is that time is not an operator in quantum mechanics, as ordinarily formulated. This prevents a canonical definition of the "uncertainty of time" Δt. In the present geometric approach this problem is solved by using the displacement between orthogonal states as the "standard" for defining Δt. The important physical result here is that the left-hand side of (27′), for arbitrary quantum evolutions between given initial and final states, must have a lower bound, and this may be interpreted geometrically as a distance or an angle.

Consider now the Schrödinger evolution of an orthonormal basis under the action of a constant Hamiltonian H which is given by a geodesic curve in the bundle $\mathscr{B}$ defined in Section 4. The projection C of this curve in $\mathscr{P}$ is the Schrödinger evolution of one of the states of this basis. Let $F_{\mu\nu}$ be the curvature of the connection in $\mathscr{B}$, regarded as a principal fiber bundle over $\mathscr{P}$, which takes its value in the Lie algebra of the structure group $U(1) \times U(N)$. By writing the geodesic equation in $\mathscr{B}$ and projecting it to $\mathscr{P}$, the equation of the curve C is obtained to be

$$\frac{dv^\mu}{ds} + \Gamma^\mu{}_{\nu\rho} v^\nu v^\rho = \frac{1}{2\,\Delta E} \operatorname{Tr}(H F^\mu{}_\nu)\, v^\nu \tag{29}$$

where $v^\mu = dz^\mu/ds = (\hbar/2\,\Delta E)(dz^\mu/dt)$ is the unit tangent vector to C which is proportional to the covariant velocity dz^μ/dt, and $\Gamma^\mu{}_{\nu\rho} = g^{\mu\bar{\alpha}}(\partial g_{\bar{\alpha}\nu}/\partial z^\rho)$ are the connection coefficients formed from the Fubini–Study metric.

Equation (29), which replaces Schrödinger's equation (1) in $\mathscr{P}$ for an isolated system, has the advantage that it is formulated in terms of the geometric quantities $g_{\mu\nu}$ and $F_{\mu\nu}$, which are obtained from the inner product in $\mathscr{H}$ and independent of the Hamiltonian H. The evolution is a geodesic if and only if H is such that the right-hand side of (29) vanishes. Equation (29) is analogous to the equation of motion of a classical particle in curved space-time in an arbitrary gauge field,[18,19] with H playing the role of the gauge field charge (color, isospin, etc.). This is the generalization of the Lorentz force law for a charged particle in an electromagnetic field to an arbitrary gauge field. In this case also, the trajectory of the particle

in space-time is the projection of a geodesic in the corresponding Kaluza–Klein space.[18]

Neither Planck's constant nor the time t, which occurs in (1), appears explicitly in (29). From (20), the Fubini–Study distance measures how far the state of the system moves from the original state as determined by its diminishing overlap with the original state. Therefore, if we measure time by the motion of a quantum system, we would directly measure the Fubini–Study distance. Time really represents the correlation between the distances measured by different systems. This is similar to how money was invented to replace what was originally a direct exchange of goods and services, which gives new meaning to the old statement that "time is money"! On the other hand, (29) is nonlinear, unlike (1). Hence, the introduction of time allows the evolution to be treated linearly.

6. MIXED STATES

There is the following profound difference between classical and quantum physics: In classical physics, if a system is in a pure state, then any part of that system is also in a pure state. But in quantum physics, the subsystem can be and usually is in a mixed state. This is because in classical physics a system is in a mixed state due to our own ignorance of the state of the system, so that we need to give a probability distribution for the possible states, e.g., a gas of molecules in classical statistical mechanics. If the state is completely known (pure state), then the state of each subsystem is also completely known. But consider now the state of two quantum systems which can always be written as

$$\sum_{k=1}^{N} c_k \, |\psi_k\rangle \, |\phi_k\rangle$$

where $|\psi_i\rangle$ and $|\phi_j\rangle$ are the states of the two individual systems satisfying $\langle\psi_i|\psi_j\rangle = \delta_{ij}$ and $\langle\phi_i|\phi_j\rangle = \delta_{ij}$. If two or more coefficients c_k are nonzero, then the combined system is said to be in an entangled state and each subsystem is in a mixed state. This is different from the mixed state for a classical system because an experiment can be performed to verify, in principle, that the combined quantum system is in a pure state and therefore we do have the maximum possible information of the combined system. This entanglement is of very great physical importance because different types of entanglements lead to Bose and Fermi statistics, the EPR paradox, and the violation of Bell's inequalities which a local realistic system should obey.

The density operators for the two subsystems are[20]

$$\rho_1 = \sum_{k=1}^{N} |c_k|^2 \, |\psi_k\rangle\langle\psi_k| \quad \text{and} \quad \rho_2 = \sum_{k=1}^{N} |c_k|^2 \, |\phi_k\rangle\langle\phi_k|$$

In the special case where only one of the coefficients is nonzero, each subsystem is in a pure state. For this to happen, it is necessary and sufficient that the density operator of either subsystem obeys $\rho^2 = \rho$. But since no system is completely isolated from its environment, a quantum system would in general be in an entangled state. It follows therefore that a description of a quantum system as a pure state is grossly inadequate and we should extend our description of the geometry of pure states given above to mixed states.

Let $\mathscr{D}$ denote the set of density operators representing the states (pure or mixed) of a given quantum system, i.e. $\mathscr{D}$ consists of the set of Hermitian operators in the Hilbert space of this system with nonnegative eigenvalues and trace equal to 1.

It is known that $\mathscr{D}$ has a topology and an affine structure with respect to which it is a convex set with the pure states contained in the boundary.[21] Since the set of pure states can be identified with the projective Hilbert space, this part of the boundary has a natural metric, namely the Fubini–Study metric. It is therefore reasonable to extend this metric to the rest of $\mathscr{D}$. To this end, write (20) in terms of the pure state density operators $\rho = |\psi\rangle\langle\psi|$ and $\rho' = |\psi'\rangle\langle\psi'|$ as

$$ds^2 = 4(1 - \mathrm{tr}(\rho\rho')) = 2\,\mathrm{tr}(\rho - \rho')^2 \tag{30}$$

where the last equality follows from $\mathrm{tr}(\rho^2) = \mathrm{tr}(\rho'^2) = 1$. It is therefore reasonable to introduce the following metric on all of $\mathscr{D}$

$$dS^2 = 2\,\mathrm{tr}(d\rho^2) \tag{31}$$

which when restricted to the pure states is the Fubini–Study metric. The metric (31) is a flat metric on $\mathscr{D}$. But its restriction to $\mathscr{P}$ has nonzero curvature because of the nonlinear condition $\rho^2 = \rho$ which defines $\mathscr{P}$ as a curved submanifold in $\mathscr{D}$.

A special case of a density operator is a "total mixture" for which ρ is of the form $\rho = (1/n)P$, where P is the projection operator which projects to a subspace of $\mathscr{H}$ of dimensions n. The set of all such ρ's, for a fixed n, may be identified with the Grassmannian $G_{n,m}$ that is defined as the set of n-dimensional subspaces of $\mathscr{H}$ whose dimension is $n+m$. This manifold has a natural metric,[22] which generalizes the Fubini–Study metric corresponding to $n = 1$, that may be defined as follows: Let $\{|\psi_k\rangle\}$ and $\{|\psi'_k\rangle\}$ be orthonormal bases in two subspaces of dimension n which are separated by an infinitesimal distance dS in $G_{n,m}$. Let $Z_{ij} = \langle\psi'_i|\psi_j\rangle$. Then

$$dS^2 = \frac{4}{n^2}(n - \mathrm{tr}\, Z^\dagger Z) = \frac{4}{n^2}(n - \mathrm{tr}\, PP') \tag{32}$$

where $P=\sum_{k=1}^{n}|\psi_k\rangle\langle\psi_k|$ and $P'=\sum_{k=1}^{n}|\psi'_k\rangle\langle\psi'_k|$ are the projection operators for the two subspaces. Hence, $dS^2=2\,\mathrm{tr}(\rho-\rho')^2$, where $\rho'=(1/n)\,P'$, which shows that (31) restricted to the submanifold of total mixtures of rank n is the usual metric (32) on $G_{n,m}$. By means of an argument similar to the one which gave (24), we have

$$\begin{aligned} dS^2 &= 4\left(\sum_{k=1}^{n}\langle d\tilde{\psi}_k|\,d\tilde{\psi}_k\rangle-\sum_{i=1}^{n}\sum_{j=1}^{n}\langle d\tilde{\psi}_i|\,\tilde{\psi}_j\rangle\langle\tilde{\psi}_j|\,d\tilde{\psi}_i\rangle\right)\\ &= 2G_{\bar{\mu}\nu}\,d\bar{Z}^{\mu}\,dZ^{\nu} \end{aligned} \tag{33}$$

where $\{|\tilde{\psi}_k\rangle\}$ is a smooth choice of orthonormal frame field in a neighborhood of $G_{n,m}$, Z^{μ} are complex coordinates in $G_{n,m}$ and the metric coefficients

$$\begin{aligned} G_{\bar{\mu}\nu} = 2\Bigg(&\sum_{k=1}^{n}\left\langle\frac{\partial}{\partial Z^{\mu}}\tilde{\psi}_k\middle|\frac{\partial}{\partial Z^{\nu}}\tilde{\psi}_k\right\rangle\\ &-\sum_{i=1}^{n}\sum_{j=1}^{n}\left\langle\frac{\partial}{\partial Z^{\mu}}\tilde{\psi}_i\middle|\tilde{\psi}_j\right\rangle\left\langle\tilde{\psi}_j\middle|\frac{\partial}{\partial Z^{\nu}}\tilde{\psi}_i\right\rangle\Bigg) \end{aligned} \tag{34}$$

It follows from (1) that the density operator ρ satisfies the evolution equation

$$i\hbar\frac{d\rho}{dt}=[H,\rho] \tag{35}$$

Therefore the velocity in $\mathscr{D}$ satisfies, from (31),

$$\left(\frac{dS}{dt}\right)^2=2\,\mathrm{tr}\left(\frac{d\rho}{dt}\right)^2=\frac{4}{\hbar^2}\,\mathrm{tr}\{(\rho^2H^2)-(\rho H)^2\} \tag{36}$$

For a pure state, (36) is the same as (26); indeed, this is a simpler derivation of this result if (31) is used as the definition of this metric. To understand the physical meaning of this result, note that the uncertainty of energy for quantum mixed state has two parts to it. There is the "classical part" which exists even when $[H,\rho]=0$, because of the energy spread of the common eigenstates of H and ρ. There is in addition a purely quantum mechanical uncertainty of energy ΔE_Q which exists merely because $[H,\rho]$ is nonzero. It is therefore reasonable to define ΔE_Q by

$$\Delta E_Q^2=-\mathrm{tr}\{[H,\rho]^2\}=2\,\mathrm{tr}\{(\rho^2H^2)-(\rho H)^2\} \tag{37}$$

Then

$$\frac{dS}{dt}=2\frac{\Delta E_Q}{\hbar} \tag{38}$$

which generalizes (26) to mixed states.

To generalize the inequality (27) to mixed states, note first that the evolution of a density operator $\rho(t)$ according to (35) lies in a submanifold $\mathscr{R}$ of $\mathscr{D}$ consisting of density operators with the same eigen values. The corresponding Cayley–Hamilton equation, which in general is non linear, is satisfied by every density operator belonging to $\mathscr{R}$. Hence, in general, $\mathscr{R}$ is a curved submanifold in $\mathscr{D}$. Clearly,

$$S \geqslant S_0 \tag{39}$$

where S is the distance along the actual evolution between the states $\rho(t_1)$ and $\rho(t_2)$ and S_0 is the distance along the shortest curve *lying entirely in* $\mathscr{R}$ joining these two states. Now $\mathscr{D}$ may be regarded as a Hilbert space with the inner product between ρ_1 and ρ_2 belonging to $\mathscr{D}$ being $2\,\mathrm{tr}(\rho_1\rho_2)$, and $\mathscr{R}$ is contained in the sphere, $2\,\mathrm{tr}(\rho^2) = \text{constant}$. Hence (39) can be rewritten, on account of (38), as

$$\int_{t_1}^{t_2} \frac{\Delta E_Q(t)}{\hbar}\, dt \geqslant \cos^{-1}(|\mathrm{tr}\{\rho(t_1)\,\rho(t_2)\}|/\mathrm{tr}\{\rho(t_1)^2\}) \tag{39'}$$

which generalizes (27′) to the space of mixed states.

7. DISCUSSION

There are two fundamental conceptions of geometry. One is Riemannian by which I mean broadly a geometry defined on a manifold by local structures such as a metric, connection, and torsion. The other is Kleinian which is the conception of Felix Klein in his Erlanger program according to which a geometry is a set of properties that are invariant under a group of transformations. The Riemannian conception of geometry is very useful in physics basically because the fundamental laws of classical physics are local. Gravity and gauge fields, classically, are described using the Riemannian conception. On the other hand, quantum mechanics is formulated in the Hilbert space of states of a quantum system on which a symmetry group acts. The state of a single particle may be regarded as a wave function on physical space, which reflects a fundamental nonlocality of quantum mechanics, particularly when a measurement is made. The success of quantum theory often appears to be due to the application of symmetries rather than the specific dynamical model used which has these symmetries. Therefore, it is the Kleinian conception of geometry which seems to be appropriate for quantum theory.[23] The task of constructing a quantum theory of gravity appears to be grounded in the problem of bringing these two conceptions of geometry together.

But the geometric structures in quantum theory described above from a Riemannian point of view may also be understood from a Kleinian point of view: The projective geometry on $\mathscr{P}$ is invariant under the group of linear transformations in $\mathscr{H}$ and may therefore be regarded physically as due to the principle of superposition. The metric on $\mathscr{P}$ is invariant under unitary and anti-unitary transformations in $\mathscr{H}$. The connection and the symplectic structure are invariant under transformations in $\mathscr{H}$ which leave invariant the imaginary part of the inner product, including unitary transformations. But they are not invariant under anti-unitary transformations, e.g., time reversal. Consequently, the geometric phase is not invariant under time reversal (it changes sign). However, all four geometric structures are invariant under the group of unitary transformations. Therefore the quantum geometry described by them is analogous to the Minkowski space-time geometry, which may also be regarded as a Riemannian geometry with zero curvature or as a Kleinian geometry invariant under the group of Poincaré transformations on space-time. Unlike for Minkowski geometry, time-reversal transformation is not a symmetry of this quantum geometry, which is interesting because time-reversal symmetry is violated in any case by weak interaction.

However, the geometric structures in $\mathscr{P}$, regarded as Riemannian structures, are "local" in $\mathscr{P}$, but not local in the sense of space-time locality which gives rise to the Riemannian space-time. Since $\mathscr{P}$ represents the physical states of the system, it is more closely related to the classical phase space rather than classical space-time. On the other hand, the classical phase space can be constructed from particle states represented on space-time which has no analog in quantum theory. That the geometry of $\mathscr{P}$ is fundamentally different from space-time geometry may also be seen from the following observation: A free classical particle moves along a geodesic in space-time. But it is neither necessary nor sufficient for a quantum particle to be free in order to move along a geodesic in $\mathscr{P}$. Therefore, it seems that there must exist a more general quantum geometry which reduces to space-time geometry when Planck's constant tends to zero. Also, from the quantum states in this geometry it should be possible to construct the above geometry in $\mathscr{P}$ when the gravitational field is negligible. Such a geometry[24] may enable us to obtain in a natural manner a quantum theory of gravity.

ACKNOWLEDGMENTS

I thank R. Penrose, R. Howard, and G. W. Gibbons for useful remarks. Part of this work was done at the University of Oxford. Also, this work was partially supported by NSF grant Nos. PHY-8807812 and INT-8912968.

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