

# Heisenberg and Isoholonomic Inequalities

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## 0.1 Introduction

A basic object in quantum mechanics is a pure state. The space of all pure states forms the projective space,  $\mathbf{P}\mathcal{H}$ , of the Hilbert space  $\mathcal{H}$  of the quantum system. The first half of this paper relates the geometry of  $\mathbf{P}\mathcal{H}$  to the quantum physics.

Most of this first half is a review of material which can be found in a recent preprint of Aharonov and Anandan [1990] and the paper [1990] of the author's. Perhaps the most striking result is a direct relation between the diameter of  $\mathbf{P}\mathcal{H}$  and Heisenberg's time-energy uncertainty relation. Another result is the "isoholonomic inequality" which is a generalization of the isoperimetric inequality. It relates the length of a closed curve in projective space to its symplectic area.

In the second half of the paper we generalize to quantum statistical mechanics. We argue that the correct replacement for the manifold  $\mathbf{P}\mathcal{H}$  of pure states is a manifold  $\mathcal{O}$  of mixed states which consists of all density matrices conjugate to an initial density matrix.  $\mathcal{O}$  is properly thought of as a co-adjoint orbit for the unitary group. We then proceed to relate the geometry of  $\mathcal{O}$  to quantum statistical mechanics. Much of this material is new. Some of it appeared in [1990] and some errors there are corrected here. The main error was that I made the wrong choice for  $\mathcal{S}$ , where  $\mathcal{S} \rightarrow \mathcal{O}$  generalizes the Hopf fibration over  $\mathbf{P}\mathcal{H}$ . The Riemannian metric on  $\mathcal{O}$  is induced from the metric on  $\mathcal{S}$  by declaring that this generalized Hopf fibration be a Riemannian submersion. Thus this mistake in  $\mathcal{S}$  led to an incorrect metric on  $\mathcal{O}$  and consequently an incorrect solution to the quantum statistical isoholonomic problem.

## 0.2 Credits

The arclength formula, equation (1) below, appeared in my paper [1990]. It was independently derived by Aharonov and Anandan [1990]. It is very likely, as remarked by Lichnerowicz remarked during my talk, that this formula has appeared elsewhere, probably several times, several decades ago, and in different guises.

The derivation of Heisenberg's uncertainty relation from this formula is due to Aharonov and Anandan [1990]. The equation for the element of phase interference is also due to Aharonov and Anandan [1987]. It is an extension of the fundamental work of Berry [1984] and Simon [1983] on the now-famous Berry's phase.

The isoholonomic inequality first appeared in my paper [1990]. That paper and indeed my interest in the subject was inspired by discussions with the physcial chemist Alex Pines and his co-workers Joe Zwanziger, Marianne Koenig, and Karl Mueller. Pines asked me "What is the shortest loop with a given holonomy?". I recommend their recent review article [1990] for more inspiration and contact with experiment.

## I.I. Overview of Part I.

We will relate the differential geometry of the manifold of pure states  $\mathbf{P}\mathcal{H}$  to the quantum physics of a system whose Hilbert space is  $\mathcal{H}$ . Recall that a point in  $\mathbf{P}\mathcal{H}$  is a one-dimensional complex subspace of  $\mathcal{H}$ . Alternatively, it is the orthogonal projection operator onto such a subspace.

The first and perhaps most important relationship which we will derive is

$$ds = \frac{\Delta E dt}{\hbar} \quad (1)$$

Here  $ds$  is the arclength along any curve in  $\mathbf{P}\mathcal{H}$  which is defined by solving Schrödinger's equation.  $\Delta E$  is the instantaneous energy uncertainty. This is the root mean square variation of the possibly time-dependent operator which defines this Schrödinger equation. And  $t$  is the time parameter of the equation. A second relationship is

$$\text{infinitesimal element of phase interference} = -\Omega \quad (2)$$

where  $\Omega$  is the Kähler form on  $\mathbf{P}\mathcal{H}$ .

These two equalities come with corresponding inequalities. The first is Heisenberg's time-energy uncertainty relation

$$(\Delta E)_{av} \Delta t \geq \frac{\hbar}{4} \quad (3)$$

where  $\Delta t$  is the duration of time of an experiment and  $(\Delta E)_{av}$  is the time average of the energy uncertainty. The second inequality is

$$L^2 \geq 2\pi\Phi - \Phi^2 \quad \text{with} \quad 0 \leq \Phi \leq 2\pi \quad (4)$$

In this inequality  $L = \int_C ds$  is the length of any closed curve  $C$  in  $\mathbf{P}\mathcal{H}$ .  $\Phi = -\int_D \Omega$  is the *symplectic area* enclosed by this curve. Thus  $D$  is any two-disc in  $\mathbf{P}\mathcal{H}$  which is bounded by  $C$  and the integral is reduced modulo  $2\pi$  to insure that  $0 \leq \Phi \leq 2\pi$ . If  $\mathcal{H} = \mathbf{C}^2$ , the Hilbert space of a two-level system, then  $\mathbf{P}\mathcal{H} = \mathbf{P}^1 = S^2$  the two-sphere of radius  $\frac{1}{2}$  and we have  $\Phi = 2(\text{Area})$ . Thus the isoholonomic inequality becomes the standard isoperimetric inequality on this two-sphere.

## I.2 Hopf Fibration

Let  $S(\mathcal{H}) \subset \mathbf{H}$  denote the unit sphere in Hilbert space. The Hopf fibration

$$\pi : S(\mathcal{H}) \rightarrow \mathbf{P}\mathcal{H}$$

is the map which assigns to each unit vector  $\psi \in \mathcal{H}$  the complex line

$$\pi(\psi) = [\psi] := \mathbf{C}\psi$$

which it spans. Alternatively, if we think of  $\mathbf{P}\mathcal{H}$  as the space of rank one projections then

$$\pi(\psi) = \psi \otimes \psi^* \quad (5)$$

### I.3. Arclength

The quantum evolution is defined by Schrödinger's equation

$$\frac{d\psi}{dt} = -\frac{i}{\hbar}H(t)\psi(t)$$

Here  $\psi(t) \in \mathcal{H}$ , the Hilbert space of the system and  $H(t)$  is the Hamiltonian of the system, a possibly time-dependent self adjoint operator on  $\mathcal{H}$ . We may take  $\mathcal{H}$  to be finite-dimensional, thus avoiding questions regarding unboundedness and domains of  $H(t)$ . However, our results appear to be true when  $\mathcal{H}$  is infinite-dimensional. The problems which originally motivated me came out of the field of nuclear magnetic resonance (NMR) in which  $\mathcal{H}$  is usually finite-dimension. If  $n$  is this finite dimension then the system is said to be an  $n$ -level system.

The self-adjointness of the Hamiltonian  $H$  implies that Schrödinger's equation preserves the norm,  $\frac{d}{dt}\langle\psi(t),\psi(t)\rangle = 0$ , thus defining a non-autonomous dynamical system on the sphere  $S(\mathcal{H})$ . Since the Hamiltonian is complex-linear it also induces a nonautonomous dynamical system on projective space: if  $C(0) = \pi(\psi(0))$  then  $C(t) = \pi(\psi(t))$  is a solution curve of of this system. Our first problem is to calculate the arclength along such a curve  $C$  of states in  $\mathbf{PH}$  in terms of the given Hamiltonian  $H$ .

In order to perform this calculation we must recall the canonical (Fubini-Study) metric on  $\mathbf{PH}$ . It is defined by declaring the Hopf map  $\pi : S(\mathcal{H}) \rightarrow \mathbf{PH}$  to be a Riemannian submersion. We recall that a submersion  $f : X \rightarrow B$  of one Riemannian manifold onto another is said to be "Riemannian" if its *restricted* differential

$$df_x : (ker(df_x))^\perp \subset T_x X \rightarrow T_{f(x)} B$$

is an isometry between the two inner product spaces. We define

$$Hor_x = (ker(df_x))^\perp$$

and call it the "horizontal space" at  $x$ . It is the orthogonal complement to the fiber  $f^{-1}(f(x))$  through  $x$ .

In our situation we put the standard metric on  $S(\mathcal{H})$ , the one induced from  $\mathcal{H}$ ,

$$ker(d_\psi\pi) = \text{real span of } i\Psi$$

and

$$T_\psi S(\mathcal{H})^\perp = \text{real span of } \Psi$$

from which it follows that

$$Hor_\psi = [\psi]^\perp \tag{6}$$

the orthogonal complement to the *complex* line through  $\psi$ . This implies that the arclength  $s$  along our curve  $C$  is given by

$$\left(\frac{ds}{dt}\right)^2 = \left\langle \frac{d\psi}{dt}^\perp, \frac{d\psi}{dt}^\perp \right\rangle$$

where

$$\frac{d\psi}{dt}^\perp = \frac{d\psi}{dt} - \left\langle \frac{d\psi}{dt}, \psi \right\rangle \psi$$

is the orthogonal projection of  $\frac{d\psi}{dt}$  onto  $Hor_\psi$ . (Our inner product convention is  $\langle\lambda\psi, v\rangle = \lambda\langle\psi, v\rangle$ .) Using Schrödinger's equation we obtain

$$\frac{d\psi}{dt}^\perp = -\frac{i}{\hbar}(H\psi - \langle H\rangle\psi)$$

where  $\langle H\rangle = \langle\psi, H\psi\rangle$  is the expected value of the energy. Now plug this in to our previous formula for  $\left(\frac{ds}{dt}\right)^2$ , take the square root and bring the  $dt$  over to the right hand side to obtain our arclength formula (1).

We take this opportunity to note that

$$\Delta E(t) = \sqrt{\sum_{i \neq 1} |H_{i1}(t)|^2}$$

where  $H_{ij}(t) = \langle \psi_i, H\psi_j \rangle$  are the matrix elements of  $H(t)$  in a (moving) orthonormal frame whose first element is  $\psi_1 = \psi(t)$ . Physically this says that  $\Delta E$  measures the amount of energy required to knock  $\psi(t)$  out of its current state  $\pi(\psi(t))$ .

When we integrate formula (1) for arclength we obtain the formula

$$L = \frac{1}{\hbar}(\Delta E)_{av}\Delta t \quad (7)$$

for the length  $L = \int ds$  of our curve  $C$ . Here  $(\Delta E)_{av} = \frac{1}{\Delta t} \int_{t_1}^{t_2} \Delta E(t)dt$  is the average energy uncertainty over the time interval  $\Delta t = t_2 - t_1$  which parameterizes  $C$ .

The distance  $d$  between two states  $p_1, p_2 \in \mathbf{PH}$  is defined as usual in Riemannian geometry

$$d(p_1, p_2) = \inf\{L(C) : C \text{ a smooth curve joining } p_1 \text{ to } p_2\}$$

and this distance is realized by a geodesic joining  $p_1$  to  $p_2$ . Every geodesic on the base space  $B$  of a Riemannian submersion  $X \rightarrow B$  is the projection of a *horizontal* geodesic on  $X$ . The general horizontal geodesic on  $X = S(\mathcal{H})$  has the form

$$\gamma(s) = \cos(s)\psi_1 + \sin(s)\psi_2 \quad \text{where} \quad \langle \psi_1, \psi_2 \rangle = 0$$

It follows immediately that the distance  $d$  between two states  $\pi(\psi)$  and  $\pi(\phi)$  is given by

$$\cos(d) = |\langle \psi, \phi \rangle| \quad , \quad \text{with} \quad 0 \leq d \leq \frac{\pi}{2} \quad (8)$$

In particular two states are orthogonal if and only if the distance between them is  $\frac{\pi}{2}$ .

#### I.4. Heisenberg's Inequality and a Review of Quantum Mechanics

We follow Aharanov and Anandan's derivation [1990] of Heisenberg's time-energy uncertainty principle from the formula for arclength. We begin by agreeing to call two states "distinguishable" if and only if they are orthogonal. We will argue this in a moment. The distance  $d$  between two distinguishable states is then  $\frac{\pi}{2}$  as we have just shown. It follows from this and equation (7) for the length of a curve that if our quantum system is evolving according to Schrödinger and if  $\pi(\psi(t_1))$ ,  $\pi(\psi(t_2))$  are two distinguishable states along the evolution curve of states then  $\frac{\Delta E_{av}\Delta t}{\hbar} \geq \frac{\pi}{2}$ . Realizing that  $\hbar = \frac{h}{2\pi}$  this becomes Heisenberg's inequality, equation (3).

We now argue the point regarding distinguishability of states. In order to do this we must recall the standard (Copenhagen) interpretation of quantum mechanics.

Measurements correspond to Hermitian operators, which we consequently call "observables". The observed values of a measurement of the observable  $A$  are its eigenvalues. The probability of observing a specific value  $a$ , given that we are in the state  $\pi(\psi)$ , is  $p(a) = \langle \mathbf{P}_a\psi, \psi \rangle$  where  $\mathbf{P}_a$  is the orthogonal projection onto  $a$ 's eigenspace. If this value of the measurement is selected then immediately after the measurement the system is no longer in the state  $[\psi]$  but instead it is in the new state  $[\mathbf{P}_a(\psi)] = \pi(\frac{\mathbf{P}_a\psi}{\|\mathbf{P}_a\psi\|})$ . (Note that the probability that  $\mathbf{P}_a = 0$  is zero.) This last fact is the mysterious "collapse of the wavepacket" phenomena. We will say that the new state is the "outcome" of the measurement of  $a$ .

We had defined two states to be "distinguishable" if and only if they are orthogonal. Now we see that this is equivalent to saying that two states are distinguishable if and only if they are possible outcomes of the measurement of some observable whose corresponding measured values are different.

For more on the topic of distinguishability of states see Datta et al [1988] and references therein. They argue that the distinguishability of non-orthogonal states leads to the instantaneous transmission of data – a la the EPR gedanken experiment – and hence to a violation of the special theory of relativity.

Aharonov and Anandan give another relation between the physics and geometry which we will take the opportunity to present now. Suppose that  $a$  is a simple eigenvalue of  $A$  and that  $\phi$  is the corresponding normalized eigenvector. Then  $\mathbf{P}_a\psi = \langle \psi, \phi \rangle \phi$  so that the probability  $p(a)$  is  $|\langle \psi, \phi \rangle|^2$ . If  $a$  is measured (and selected, as in the Stern-Gerlach experiment, for instance) then we are in the state  $\pi(\phi)$ , so that we can call  $p = p(a)$  the "probability of the transition"  $\psi \rightarrow \phi$ . It follows from equation (8) that the distance  $d$  and transition probability  $p$  between two states are related by

$$d = \arccos(\sqrt{p})$$

## I.5 Phases and Holonomy

Formula (6) defines the horizontal distribution for the canonical connection on the Hopf fibration. The corresponding connection one-form is

$$\Gamma(\psi) = -\Im\langle\psi, d\psi\rangle$$

where “ $\Im$ ” is plain TeX’s funny way of saying “the imaginary part of”. Its curvature form  $\Omega$  is the Kähler form on  $\mathbf{P}\mathcal{H}$  :

$$\pi^*\Omega = d\Gamma$$

Suppose now that our curve  $C(t) = \pi(\psi(t))$  is periodic with period  $\Delta t$ . Then

$$\psi(t_2) = \exp(i\Delta\theta)\psi(t_1)$$

for some phase factor  $\Delta\theta$  defined modulo  $2\pi$ . There is a formula this phase factor.

$$\Delta\theta = -\int_D \Omega - \frac{E_{av}\Delta t}{\hbar}$$

The surface integral is over any disc  $D$  which bounds  $C$  and  $E_{av} = \frac{1}{\Delta t} \int_{t_1}^{t_2} E(t)dt$  is the average of the expected energy  $E(t) = \langle\psi(t), H(t)\psi(t)\rangle$ , around the loop  $C$ .

This formula is Aharonov and Anandan’s generalization [1987] of Berry’s [1983] phase formula. It is easy to derive, being just the integrated version of the decomposition of  $\frac{d\psi}{dt}$  into horizontal and vertical parts. For details see Aharonov and Anandan [1987] or the author [1990], section 3. If  $E_{av} = 0$ , then we get

$$\Delta\theta = -\int_D \Omega$$

which is the integrated version of formula (2) for the element of “phase interference”.

## I.6 Isoholonomic Inequality

From the work thus far it follows that the two questions, “What is the shortest loop in  $\mathbf{P}\mathcal{H}$  with a given holonomy?” and “How can we obtain a desired phase shift with the least average fluctuation in energy?” are the same, provided the average energy of the loop is zero. The physical chemist Alex Pines posed this question to me and in [1990] I solved it. I called the loops which solve this question “isoholonomic curves”.

To describe these isoholonomic curves first consider the case  $\mathcal{H} = \mathbf{C}^2$ . Then  $\mathbf{P}\mathcal{H} = S^2$ , the two-sphere of radius  $\frac{1}{2}$ , and the Kähler form is the area form. Therefore our question is the classical isoperimetric problem, “What is the shortest loop enclosing a fixed area?”, the answer to which is well-known. The solutions are geometric circles on the surface of the sphere.

Every such circle enjoys the following properties.

- (1) It is the image under the Hopf projection of a geodesic in  $S(\mathcal{H})$ .
- (2) It is itself a geodesic (i.e. a great circle) if and only if the corresponding geodesic in  $S(\mathcal{H})$  is *horizontal*.
- (3) It can be generated by a *time-independent* Hamiltonian.
- (4) Its length and (spherical) area are related by  $L^2 = 4\pi A - 4A^2$ . ( $K = 4$  is the curvature of the sphere.)

Note in this last equality that it does not matter which of the two areas bounded by the circle are taken; the answer is the same.

I showed in [1990] that these properties (1)-(3) hold for the isoholonomic solution curves for a general Hilbert space. In fact, every such solution lies on some  $S^2 = \mathbf{P}V \subset \mathbf{P}\mathcal{H}$  for some two-dimensional subspace  $V$  of  $\mathcal{H}$  and is a isoholonomic minima, and thus a geometric circle, for the restricted bundle-with-connection  $S(V) \rightarrow \mathbf{P}V$ . As for the final property (4), the symplectic area

$$\Phi = -\int_D \Omega$$

is independent modulo  $2\pi$  of the choice of disc  $D$  bounded by  $C$ . Since the isoholonomic minima are geometric circles on some  $\mathbf{P}V$  and since on this  $\mathbf{P}V$  we have  $\Omega = -2$  (area form) and the equality in property (4), we have demonstrated the validity of the Isoholonomic inequality (4), in the following sharp form. For any loop  $C$  on  $\mathbf{P}\mathcal{H}$  with length  $L$  and enclosing a symplectic area  $\Phi$  with  $0 \leq \Phi \leq 2\pi$  the inequality

$$L^2 \geq 2\pi\Phi - \Phi^2$$

holds, with equality if and only if  $C$  is a geometric circle lying on some projective line  $\mathbf{P}^1$  within  $\mathbf{P}\mathcal{H}$ .

### I.7. Measuring Holonomy

In this section we will discuss methods for experimentally measuring holonomy. For further questions I recommend the review article by Zwanziger et al [to appear 1990].

Overall phase changes cannot be detected because experimental data, namely averages and probability distributions of measurements, are invariant under global phase changes  $\psi \rightarrow e^{i\theta}\psi$ . Only *relative phase changes* are measurable. This means that to observe holonomies the experimentalist must prepare a *superposition* of states.

Suppose that the normalized vector  $\psi_1$  undergoes a projective cycle:  $C_1(t) = \pi(\psi_1(t))$  under the influence of the Hamiltonian  $H(t)$  and that another normalized vector  $\psi_2$  undergoes a (different) projective cycle  $C_2(t)$  of the same period  $T$ . Let  $\Delta\theta_i = \gamma_i + \frac{E_i T}{\hbar}$ ,  $i = 1, 2$  be the corresponding phases accumulated by the  $\psi_i$  during their cycles. The  $\gamma_i$  are the symplectic areas, i.e. the logarithms of the holonomies, of the loops. The  $E_i$  are their average expected energies. Now prepare the superposition

$$\psi = a\psi_1 + b\psi_2 \quad \text{with} \quad |a|^2 + |b|^2 = 1$$

and measure some observable  $M$ . After  $k$  periods the average value of the measurements will be

$$\langle \psi(kT), M\psi(kT) \rangle = A + B \cos\{k(\Delta\theta_1 - \Delta\theta_2) + \theta_0\}$$

where  $A$ ,  $B$ , and  $\theta_0$  are constants independent of the number of periods  $k$ . (For example  $A = |a|^2 \langle \psi_1, M\psi_1 \rangle + |b|^2 \langle \psi_2, M\psi_2 \rangle$ .) In the particular case where  $E_1 = E_2$  we have  $\Delta\theta_1 - \Delta\theta_2 = \gamma_1 - \gamma_2$  and so the *difference* of the (logarithms) of the holonomies appears as the *frequency* of oscillation of observables.

In NMR experiments the  $x$ -component,  $M = M_x$ , of the bulk magnetization of a sample is measured as a function of a *frequency*  $\omega$ . This frequency is related to the time  $t$  or  $kT$  by Fourier transform. The net result is that the difference of holonomies manifests itself as a shift (and perhaps a splitting) of a particular line (=peak) in the NMR spectrum (graph of  $M$  vs.  $\omega$ ).

Most (perhaps all to date) experiments measure the relative holonomies of pairs of curves with one of the two following types of geometries.

The first geometry consists of two curves for a two-level system. Thus  $\mathbf{P}\mathcal{H} = S^2$  is the standard two-sphere in  $\mathbf{R}^3$ . The initial states  $\psi_1$  and  $\psi_2$  are prepared so as to be perpendicular to each other. This is equivalent to  $\pi(\psi_2)$  being antipodal to  $\pi(\psi_1)$  on the two-sphere. The two states remain antipodal,  $C_1(t) = -C_2(t)$ , since the evolution is unitary. The antipodal map is orientation reversing so that the two symplectic areas are negatives of each other. Consequently the observed frequency shift  $\gamma_1 - \gamma_2$  will be the negative of the solid angle enclosed by  $C_1$ . This is the type of geometry incorporated in the NMR experiments of Tyko [1987], the optical experiments of Tomita and Chiao [1986], and the neutron interferometry experiments of Bitter and Dubbers [1987].

The second type of geometry concerns three-level systems so that  $\mathbf{P}\mathcal{H} = \mathbf{P}^2$ .  $C_1$  lies entirely inside a two-level subsystem and  $C_2$  is the constant state which represents the third level orthogonal to this subsystem. Thus  $\gamma_2 = 0$  and the observed frequency shift will be  $\gamma_1 - \gamma_2 = -\int_{D_1} \Omega$ . This is the type of geometry tested in the experiment performed by Suter, Mueller, and Pines [1988].

There is a nice projective interpretation for this second type of experiment.  $\mathcal{H} = \mathbf{C}^2 \oplus \mathbf{C}$  and the first curve travels in  $\mathbf{P}^1 = \mathbf{P}(\mathbf{C}^2) \subset \mathbf{P}\mathcal{H} = \mathbf{P}^2$ . The normal bundle  $N$  of  $\mathbf{P}^1$  is naturally isomorphic to the tautological line bundle over  $\mathbf{P}^1$ . This is the line bundle whose unit vectors forms the Hopf fibration  $S^3 \rightarrow \mathbf{P}^1$ . When we prepare a superposition of  $\psi_1$  and  $\psi_2$  we move off of the zero-section,  $\mathbf{P}^1 \subset N$ , and onto some non-zero vector  $\pi(a\psi_1 + b\psi_2) \in N$ . This vector evolves under Schrödinger as the *horizontal lift*

of  $C_1$  with respect to the natural connection on the tautological line bundle, and it is the logarithm of this holonomy which is measured.

## Part II. Geometry of Mixed States

### II.1 Overview

In this half of the paper we will see what happens to the relationship between physics and geometry when we replace quantum mechanics by quantum statistical mechanics. The basic objects are now density matrices. These can be thought of as elements in the dual,  $u(\mathcal{H})^*$ , of the Lie algebra of the unitary group,  $U(\mathcal{H})$ . Our replacement for  $\mathbf{PH}$  is the set  $\mathcal{O} = \mathcal{O}(\rho)$  of all density matrices conjugate to a given density matrix  $\rho$ . In other words,  $\mathcal{O}$  is the *co-adjoint orbit* through  $\rho$ .

Our arclength formula (1) no longer holds generally but it still holds for *horizontal* Schrödinger evolutions. The element of arclength on  $\mathcal{O}$ , and the connection (choice of horizontal) over  $\mathcal{O}$  are still defined by declaring that a certain bundle projection  $S \rightarrow \mathcal{O}$  is a Riemannian submersion. **Our main achievement here is the correct choice for the Riemannian manifold  $S$** , the quantum statistical replacement for  $S(\mathcal{H})$ . We define  $S$  to be the fiber bundle over  $\mathcal{O}$  whose fiber  $S_\rho$  over  $\rho$  consists of the set of orthogonal ( *not orthonormal!* ) frames,  $\{\phi_i\}_{i=1, \dots, \text{rank}(\rho)}$ , of eigenvectors for  $\rho$ . Thus  $\rho\phi_i = c_i\phi_i$  (no sum) where the  $c_i$  are  $\rho$ 's nonzero eigenvalues listed in (say) decreasing order. The normalization for the frames is according to these eigenvalues:

$$\langle \phi_i, \phi_j \rangle = c_i \delta_{ij} \quad (\text{no sum})$$

$S$  sits inside the Hilbert space  $k\mathcal{H}$ , the direct sum of  $k = \text{rank}(\rho)$  copies of  $\mathcal{H}$ . Its Riemannian metric is the one induced from this embedding.

$S \rightarrow \mathcal{O}$  forms a principal bundle which we will sometimes call the "generalized Hopf fibration". Its structure group  $G = G(\rho)$  is the commutant of  $\rho$ , that is, the group of all unitaries which commute with  $\rho$ . The phase associated to a loop in  $\mathcal{O}$  is thus the logarithm of an element of  $G$ . There is no "non-Abelian Stoke's formula"; consequently there is no simple formula such as Berry's for this phase in case  $G$  is non-Abelian. This much is well-known.

In the past authors (including myself) have chosen the frames comprising  $S$  to be orthonormal. This corresponds to inducing the metric on  $S$  from the bi-invariant metric on  $U(\mathcal{H})$ . There are at least two other well-known Riemannian metrics on a coadjoint orbit  $\mathcal{O}$  of  $U(\mathcal{H})$  for which  $U(\mathcal{H})$  acts by isometries. One of these is the induced metric, that is the one obtained by viewing the orbit as a submanifold of the Euclidean space formed by the (dual) Lie algebra. The other is the Kähler metric. This is the real part of the Kähler structure whose imaginary structure is the (Kirillov-Kostant-Souriau) symplectic structure. I claim that none of these choices are "correct" from the quantum statistical point of view. The correct metric is obtained by Riemannian submersion from the above described eigenbundle  $S$ . An argument for why this is correct appears in §II.5.

## II.2 : Review of Quantum Statistical Mechanics. The Generalized Hopf Fibration

I will now give a very brief review of the formalism of quantum statistical mechanics. See the books of Feynman (1972) and of Mackey (1963) for a more complete picture. In this review I completely ignore most of the central concepts such as the Boltzman distribution and temperature. The main goal is to convince you that the correct replacement for  $\mathbf{PH}$  is  $\mathcal{O}$ . We will also describe the generalized Hopf fibration  $S \rightarrow \mathcal{O}$  in more detail.

Observables in quantum statistical mechanics are self-adjoint operators on  $\mathcal{H}$ , the same as in the standard non-relativistic mechanics. A *state* in quantum statistical mechanics is a non-negative Hermitian matrix  $\rho$  with trace one

$$\rho = \rho^* \quad \rho \geq 0 \quad tr(\rho) = 1$$

A state is also called a “density matrix” or a “mixed state”. We can always express a state in the form

$$\rho = c_1 \psi_1 \otimes \psi_1^* + c_2 \psi_2 \otimes \psi_2^* + \dots \quad (II.1a)$$

with

$$c_i > 0 \quad , \quad \sum c_i = 1 \quad , \quad \text{and the } \psi_i \text{ an orthonormal frame} \quad (II.1b)$$

The  $c_i$  are of course the non-zero eigenvalues of  $\rho$ . The state is called “pure” if there is only one  $c_i$ , in which case it is  $c_1 = 1$  and  $\rho$  has rank 1.

The set  $\mathcal{S}$  of all states forms a convex bounded subset within the real vector space of all Hermitian matrices. Its extreme points are formed by the set  $\mathcal{S}_{pure}$  of pure states. Moreover

$$\mathcal{S}_{pure} = \mathbf{PH}$$

with the identification map being defined by equation (5). In this manner, standard quantum mechanics is embedded in the quantum statistical mechanics.

If  $A$  is a bounded observable then  $tr(\rho A)$  is its “expected value” relative to the state  $\rho$ . The assignment  $A \mapsto tr(\rho A)$  is a positive (  $A \geq 0 \Rightarrow tr(\rho A) \geq 0$  ) normalized (  $tr(\rho 1) = 1$  ) linear functional on the space of bounded observables. Thus our states are states in the  $C^*$ -algebra sense, for the  $C^*$ -algebra  $\mathcal{B}(\mathcal{H})$  of all bounded operators on  $\mathcal{H}$ .

We will henceforth identify the space of bounded observables, a real linear subspace of  $\mathcal{B}(\mathcal{H})$ , with the Lie algebra  $u(\mathcal{H})$  of all skew-hermitian operators in the standard fashion: multiplication by  $i$ . Thus the set of states  $\mathcal{S}$  forms a subset of  $u(\mathcal{H})^*$ , the dual of the Lie algebra of the unitary group. This subset is clearly invariant under the (co-) adjoint action  $\rho \mapsto g \rho g^*$ .

The quantum evolution of a state is defined by the equation

$$\frac{d\rho}{dt} = \frac{i}{\hbar} [\rho(t), H(t)]$$

which sometimes goes under the name of Liouville’s equation. It looks just like Heisenberg’s equation except for a sign change due to the fact that states transform contragrediently with respect to observables.  $H(t)$  is the same as before: a time-dependent observable. These equations imply that

$$\rho(t) = g(t) \rho(0) g(t)^*$$

where  $g(t)$  is a unitary matrix (called the “propagator” or fundamental solution). Consequently  $\rho$  remains on whatever co-adjoint orbit it began on.

This co-adjoint orbit is completely specified by  $\rho$ ’s non-zero eigenvalues. From now on we assume that

$$k = rank(\rho) < \infty$$

for simplicity. Let  $\mathbf{c} = (c_1, c_2, c_3, \dots, c_k)$  be the list of these eigenvalues, including multiplicity, and in increasing order:  $c_1 \geq c_2 \geq c_3 \dots$ . Then the co-adjoint orbit is specified as

$$\mathcal{O}(\mathbf{c}) = \{ \rho \in \mathcal{S} : \text{the nonzero spectrum of } \rho = \{\mathbf{c}\} \}$$



Of course, when we say “nonzero spectrum” we mean to include the information of multiplicities.

The spaces  $\mathcal{O}(\mathbf{c})$  are the generalizations of  $\mathbf{PH} = \mathcal{O}(1)$ . The generalization of  $S(\mathcal{H})$  is

$$S(\mathbf{c}) = \{(\phi_i) : (\phi_i) \text{ is an orthogonal frame in } \mathcal{H} \text{ normalized according to } \langle \phi_i, \phi_j \rangle = c_i \delta_{ij}\}$$

as we said earlier. The number of elements in each such frame is  $k =$  the rank of  $\rho$ . The generalized Hopf projection is

$$\pi(\phi_1, \phi_2, \dots) = \sum \phi_i \otimes \phi_i^* \tag{II.2}$$

To relate this to equation (II.1a) for  $\rho$ , set  $\phi_i = \sqrt{c_i} \psi_i$ . In the final section I argue that this is the correct generalization of the Hopf fibration.

Let  $c(1) = c_1 < c(2) = c_{m(1)+1} < \dots$  be  $\rho$ 's positive eigenvalues listed *without* multiplicities and let  $m(i)$  be their corresponding multiplicities. Thus

$$\begin{aligned} \sum m(i)c(i) &= 1 \\ \sum m(i) &= k \end{aligned}$$

$\pi : S(\mathbf{c}) \rightarrow \mathcal{O}(\mathbf{c})$  is a principal bundle with structure group

$$G(\mathbf{c}) = U(m(1)) \times U(m(2)) \times \dots$$

a product of unitary groups.

**Example 1**  $G(1) \rightarrow S(1) \rightarrow \mathcal{O}(1)$  is our friend the standard Hopf fibration.

**Example 2**  $G(\frac{1}{k}, \frac{1}{k}, \dots, \frac{1}{k}) \rightarrow S(\frac{1}{k}, \frac{1}{k}, \dots, \frac{1}{k}) \rightarrow \mathcal{O}(\frac{1}{k}, \frac{1}{k}, \dots, \frac{1}{k})$  is the bundle of  $k$ -frames, also known as the Steiffel variety (except that our frames are normalized to be smaller). Its fiber is  $U(k)$  and the base space is the Grassmannian of all  $k$ -planes in  $\mathcal{H}$ .

$S(\mathbf{c})$  inherits a Riemannian structure as a sub-manifold of  $k\mathcal{H} = \mathcal{H} \oplus \dots \oplus \mathcal{H}$  ( $k$  times). Now  $U(\mathcal{H})$  and  $U(k)$  act by isometries on  $k\mathcal{H} = \mathcal{H} \otimes \mathbf{C}^k$ .  $U(\mathcal{H})$  and  $G(\mathbf{c}) \subset U(k)$  leave  $S = S(\mathbf{c})$  invariant and so act on it by isometries. The fibers of  $\pi : S \rightarrow \mathcal{O}$  are the  $G(\mathbf{c})$ -orbits. This allows us to put a metric on  $\mathcal{O}$  by declaring  $\pi$  to be a Riemannian submersion. We also get a connection on the bundle in this manner. (See the paragraph on Riemannian submersions near the beginning of the paper.)

With this structure of a Riemannian submersion in place, we can address all of the questions which we previously answered for  $\mathbf{PH}$ . What is the (quantum statistical) meaning of the element of arclength on  $\mathcal{O}$ ? Of the holonomy of a loop? How do we measure the holonomy? What is the shortest loop with a given holonomy? We will only address the first and last question.

### II.3 Arclength

We begin by fixing  $(c_1, c_2, \dots) = \mathbf{c}$  and abbreviate  $S(\mathbf{c}) = S$ , and similarly for  $\mathcal{O}$  and  $G$ .  $U(\mathcal{H})$  acts transitively on  $S$  so that any tangent vector to  $S$  at  $\phi = (\phi_1, \phi_2, \dots)$  can be written

$$\left(\frac{d\phi}{dt}\right)_j = \frac{\sqrt{-1}}{\hbar} H\phi_j$$

for some self-adjoint operator  $H$  independent of the index  $j$ . This is to say, every tangent vector can be realized by some Schrödinger evolution. The squared length of this vector is

$$\begin{aligned} \left\|\left(\frac{d\phi}{dt}\right)\right\|^2 &= \sum \left\|\frac{d\phi_j}{dt}\right\|^2 \\ &= \frac{1}{\hbar^2} \sum \langle H\phi_j, H\phi_j \rangle \\ &= \frac{1}{\hbar^2} \sum \langle \phi_j, H^2\phi_j \rangle \\ &= \frac{1}{\hbar^2} \text{tr}(\rho H^2) \end{aligned}$$

where  $\rho = \pi(\phi)$  is the density matrix corresponding to the frame  $\phi$ . The last line in this column of equalities follows from the general fact  $\text{tr}(\rho A) = \sum \langle \phi_j, A\phi_j \rangle$ . We can re-express this equation in the form

$$ds_S = \frac{dt}{\hbar} \sqrt{\langle H^2 \rangle_\rho} \quad (II.3)$$

Polarizing this formula we obtain the curious inner product formula

$$\langle iH_1(\phi), iH_2(\phi) \rangle_\phi = \frac{1}{\hbar^2} \text{tr}(\rho [H_1, H_2]_+)$$

where  $iH(\phi)$  denotes the vector at  $\phi$  generated by the Hamiltonian  $H$  and where  $[H_1, H_2]_+ = H_1H_2 + H_2H_1$  denotes the anti-commutator.

We need to know the horizontal projection  $T_\phi S \rightarrow (\ker T_\phi \pi)^\perp$  in order to calculate the arclength on  $\mathcal{O}$ . The vertical projection  $T_\phi S \rightarrow (\ker T_\phi \pi)$  is

$$\delta\phi_j \mapsto \mathbf{P}_j(\rho)\delta\phi_j$$

where  $\mathbf{P}_j(\rho) : \mathcal{H} \rightarrow \mathcal{H}$  is the orthogonal projection onto  $c_j$ 's eigenspace. The horizontal projection is 1-(this). In particular, if  $\phi \in S$  evolves according to Schrödinger and is also a horizontal curve, then  $\mathbf{P}_j(\rho)\frac{d\phi_j}{dt} = \mathbf{P}_j H\phi_j = 0$ . Then  $\langle \phi_j, H\phi_j \rangle = 0$  so that  $\text{tr}(\rho H) = 0$ . This yields our formula (1):

$$ds_{\mathcal{O}} = \frac{dt}{\hbar} (\Delta E)$$

provided that the evolution on  $S$  is by a horizontal Schrödinger evolution. For the case  $\mathcal{O} = \mathbf{P}\mathcal{H}$  of part I we did not need to add the adjective "horizontal".

For a general Schrödinger evolution the element of arclength can be expressed as

$$ds_{\mathcal{O}}^2 = \frac{dt^2}{\hbar^2} (\langle H^2 \rangle - \sum \langle \phi_j, H\mathbf{P}_j H\phi_j \rangle)$$

which is typically not equal to our previous expression for  $ds_{\mathcal{O}}$  squared. In fact, no matter how the metric on  $\mathcal{O}$  is chosen,  $ds_{\mathcal{O}} \neq \frac{dt}{\hbar} (\Delta E)$  for general Schrödinger curves. This is because given any impure state  $\rho$  there exist  $H$ 's which represent the zero-tangent vector to  $\mathcal{O}$ , i.e. for which  $[\rho, H] = 0$ , but for which  $\Delta E_\rho \neq 0$ .

A perhaps more illuminating formula for  $ds_{\mathcal{O}}$  can be obtained by writing  $H$  in block form with respect to the eigenspaces  $E(i)$  of the  $c(i)$ . (Recall that these are the eigenvalues listed without multiplicity.) Thus  $H_{(ij)} = \mathbf{P}_j H \mathbf{P}_i : E_i \rightarrow E_j$  is an  $m(i) \times m(j)$  matrix. We must also include blocks for the 0-eigenspace  $E_0$  of  $\rho$ . We do this by adding an extra index 0 with  $c(0) = 0$ . Then one calculates that

$$\left(\frac{ds_{\mathcal{O}}}{dt}\right)^2 = \frac{1}{\hbar^2} \sum_j c(j) \sum_{k \neq j} \text{tr}(H_{(jk)} H_{(kj)})$$

In words, the squared length is a weighted sum of the squared lengths of the *off-diagonal* blocks of the Hamiltonian, the weights being  $\rho$ 's eigenvalues. As in part I, this arclength is a measure of the amount of energy required to change the current state to a new state.

It is illuminating to rewrite this formula:

$$(ds_{\mathcal{O}})^2 = \frac{1}{\hbar^2} \sum_{j>k} (c(j) + c(k)) \text{tr}(H_{(jk)} H_{(kj)}) (dt)^2$$

and then to compare it with the formula

$$(ds_{\mathcal{O}, \text{Kahler}})^2 = \frac{1}{\hbar^2} \sum_{j>k} (c(j) - c(k)) \text{tr}(H_{(jk)} H_{(kj)}) (dt)^2.$$

This last formula is the formula for the Riemannian metric on  $\mathcal{O}$  obtained by taking the real part of the corresponding Kähler metric, the one whose imaginary part is the natural (Souriau-Kostant-Kirillov) symplectic form on this co-adjoint orbit. See, for example, Besse.

As an example of this formula consider the case of the Grassmannian of  $k$ -planes, example 2 above. Then  $\rho = \frac{1}{k} \mathbf{P}$  where  $\mathbf{P}$  is a rank  $k$  projection operator.  $H$  is a  $2 \times 2$  block matrix and

$$ds_{\mathcal{O}}^2 = \frac{1}{k\hbar^2} \text{tr}(H_{(12)} H_{(21)})$$

where  $H_{(12)} = \mathbf{P}H(1 - \mathbf{P})$  and  $H_{(21)} = H_{(12)}^*$  are the two off-diagonal blocks.

### Phases and Curvature

There is no simple formula for the holonomy of a loop on  $\mathcal{O}$ . This is because there is no non-Abelian Stokes formula. However in the special case where  $G$  is Abelian, that is where all the  $c_i$  are distinct, there is a Stoke's formula.

The curvature of the connection can be calculated in terms of operator-valued forms. See Avron, Sadun, Segert and Simon [1988]. The result is

$$\Omega = \sum P_i (dP_i) \wedge (dP_i) P_i$$

where  $P_i : \mathcal{O} \rightarrow u(\mathcal{H})$  is the projection-valued function which assigns to each density matrix  $\rho \in \mathcal{O}$  the projection  $P_i(\rho)$  onto the eigenspace for  $c(i)$ .

## The Isoholonomic Problem and Some Corrections to the Literature.

In [1990] I partially characterized the isoholonomic minimizers for  $\pi : \mathbf{S} \rightarrow \mathbf{O}$ . In this subsection we will review and **correct** this characterization.

In the general setting of Riemannian submersions it is simpler to try to characterize the **isoparallel extremals** instead of the isoholonomic minima. “Parallel” as opposed to “holonomic” because we will not be able to say that the curve on  $\mathbf{O}$  is closed. (For a non-closed curve  $\gamma$  in  $\mathbf{O}$  what we fix instead of the holonomy is the parallel translation map which is a  $G$ -automorphism from the fiber over the initial point  $\gamma(t_1)$  to the fiber over the final point  $\gamma(t_2)$ . Alternatively, we fix the end points of the horizontal lift  $\tilde{\gamma}$  of  $\gamma$ .) “Extrema” as opposed to “minimal” because we will only say that  $\tilde{\gamma}$  extremizes length among all horizontal curves with these endpoints.

We will now state the analogues of properties (1) through (4) of the section “Isoholonomic Inequality” of part I. After the statements, we will discuss various errors which occurred in my previous paper[1990].

(1’) Any projected geodesic from  $\mathcal{S}$  is an isoholonomic extremal on  $\mathcal{O}$ . For sufficiently small subarcs these extremals are isoholonomic minima.

(2’) An isoparallel extremal is a geodesic on  $\mathcal{O}$  if and only if it is the projection of a horizontal geodesic on  $\mathcal{S}$ .

(3’): “Every isoparallel extremal is generated by a time-independent Schrödinger equation ” is **simply false** for typical  $\mathcal{S} \rightarrow \mathcal{O}$ .

(1’) and (2’) are true for any Riemannian submersion **provided the fiber metric is covariantly constant**.

In [1990] and in my lecture I incorrectly stated that the converse to (1’) holds in the general setting of Riemannian submersions. (I was quoting a theorem of another author.) But very recently I have found a counterexample to this alleged converse, that is, an isoparallel **minimum** which is not the projection of any geodesic from the total space. In this counterexample the Hörmander condition holds everywhere: the image of the curvature form together with all of its covariant derivatives spans the Lie algebra of  $G$ . In the example one more covariant derivative is needed for points over the counterexample curve in comparison to all other points. Such “pathologies” occur in our generalized Hopf fibrations but it is still possible that the converse to (1’) holds here. I do not know.

In [1990] I made the statement in quotes in (3’). My mistake was that I used the wrong metric on  $S$ . (I used a metric induced by Riemannian submersion from a bi-variant metric on  $U(H)$ .)

To see that this statement in quotes in (3’) is false, we note that the time-independent Schrödinger equation defined by  $H$  generates a geodesic in  $S$  **if and only if**

$$[\rho, H^2] = 0$$

But a dimension count shows that this last condition typically constrains the set of geodesic-generating  $H$ ’s to be smaller than the set of directions at  $\varphi$ . (If all the  $c_i$ ’s are distinct the dimension count yields dimension zero, so a finite set of directions.) Our claim follows: for typical  $S$  there are geodesics, and hence isoparallel extremals, which are not generated by any autonomous Schrödinger equation.

Regarding our statement concerning the condition  $[\rho, H^2] = 0$ . A curve  $\varphi(t)$  in  $S$  is a geodesic if and only if  $\frac{d^2\varphi}{dt^2} \perp T_\varphi S$ . A direct calculation similar to our arclength calculation shows that this in turn is true if and only if  $[\rho, H^2] = 0$ , provided, of course, that the  $\varphi(t)_j$ ’s evolve according to Schrödinger for this  $H$ .

## II.5 How to use Dual Paris to Ignore the Rest of the Universe

In this final section we will construct the bundle  $S \rightarrow \mathcal{O}$  using symplectic reduction. This provides evidence that our bundle and in particular our normalization of the frame  $\varphi \in S$  is the correct choice, both from the points of view of physics and of geometry.

A standard argument for the necessity of statistical mechanics proceeds as follows. (See for example, Feynman [1972] Chapter 2.) When we analyze any system we necessarily separate it from the rest of the universe. But the true description involves the rest of the universe. Statistical mechanics provides a means for systematically ignoring the rest of the universe while still providing a reasonably accurate picture of the system of interest.

Restated in the formalism of quantum mechanics this argument begins as follows. The Hilbert space for the universe splits as a tensor product:

$$\mathcal{H}_u = \mathcal{H} \otimes \mathcal{H}_r$$

Here  $\mathcal{H}$  is the Hilbert space of the system of interest and  $\mathcal{H}_r$ , "r" for "rest", is the Hilbert space for the rest of the universe. (Recall that in quantum mechanics when two systems are coupled we take their tensor product, not their direct sum.) Alternatively, simply set  $\mathcal{H}_u = k\mathcal{H} = \mathcal{H} \otimes \mathbf{C}^k$  of the previous section and interpret  $\mathbf{C}^k$  as the rest of the universe.

We require a method for ignoring all of the extraneous or perhaps inaccessible information in  $\mathcal{H}_r$ . Given the nature and participants of this conference, there is really only one possible method to use: symplectic reduction!

The group to reduce by is  $U(\mathcal{H}_r) = U_r$ . It acts transitively on the set of directions in  $\mathcal{H}_r$ , and so reduction by its action should get rid of all  $\mathcal{H}_r$  information.

$U(\mathcal{H}) = U$  and  $U_r$  form a Howe dual pair within the large group  $Sp(\mathcal{H}_u)$  of all real-linear symplectic transformations of  $\mathcal{H}_u$ . This means that they are reductive and are each other's commutants within the large group. Our pair of groups  $(U, U_r)$  also satisfy an additional technical property labeled (Q) below. Any dual pair enjoying property (Q) has the following remarkable property. *Every symplectic reduced space for one group is isomorphic to the closure of a co-adjoint orbit in the dual of the other group's Lie algebra.* In our case this means that our mixed-state manifolds  $\mathcal{O}(\rho)$  are reduced spaces for this action of  $U_r$  on  $\mathcal{H}_u$ .

To be honest, the italicized statement above is only known to be true when one element of the dual pair is compact and when this is the group by which we are reducing. This was proved recently by Lerman, Montgomery, and Sjamaar [1991]. (I suspect it is true for general Howe pairs.) The reason the proof is so recent is that it requires the machinery of stratified symplectic reduction to make sense of the possibly singular reduced space. This machinery was developed very recently by Sjamaar and Sjamaar-Lerman.

In any case, for our dual pair, both elements are compact. For this reason there is also no need to take the closure in the italicized statement above: orbits are already closed.

We now outline the correspondence "orbits  $\leftrightarrow$  reduced spaces" for a general dual pair  $(G, G_r)$  within  $Sp(E)$ , where  $E$  is a symplectic vector space. For more on dual pairs see Kazhdan, Kostant and Sternberg [1978] Our particular dual pair appears on the last page of their article.

Write down the momentum maps,  $J_r$  and  $J$ , for the two groups :

$$Lie(G_r)^* \longleftarrow E \longrightarrow Lie(G)^*$$

Take  $\rho \in Lie(G)^*$  with the property that there is a  $\varphi \in E$  with  $J(\varphi) = \rho$ . Construct the reduced space:

$$M_{\mathbf{c}} := J_r^{-1}(\mathbf{c}) / (G_r)_{\mathbf{c}}$$

for

$$\mathbf{c} = J_r(\varphi)$$

Here  $(G_r)_{\mathbf{c}}$  denotes the isotropy group of  $\mathbf{c}$ . Since the  $G$  and  $G_r$  actions on  $E$  commute,  $J$  is a  $G_r$ -invariant map. It follows that the map  $J$ , upon restriction to  $J_r^{-1}(\mathbf{c})$ , induces a map

$$i_{\mathbf{c}} : M_{\mathbf{c}} \longrightarrow \mathcal{O}(\rho)$$

whose the target is the co-adjoint orbit through  $\rho$ . It maps onto  $\mathcal{O}$  because  $J_r$  is  $G$  - invariant so that  $G(J_r^{-1}(\mathbf{c})) = J_r^{-1}(\mathbf{c})$ .

We need to know when  $i_{\mathbf{c}}$  is one-to-one. This is where the technical property (Q) comes in . The epimorphism  $i_{\mathbf{c}}$  is one-to-one iff any  $G_r$  - invariant functions on  $E$  can be expressed as a smooth function of the components of  $J$ . (Recall that the reduced space is isomorphic to  $J_r^{-1}(G_r\mathbf{c})/G_r$ .) The fact that  $G$  and  $G_r$  form a dual pair implies that every quadratic form on  $E$  which is invariant under  $G_r$  can be expressed in terms of the components of  $J$  which are themselves homogeneous invariant quadratic polynomials on  $E$ . (Identify the Lie algebra of  $Sp(E)$  with the space of homogeneous quadratic functions on  $E$ .) Thus we need to know whether are not these are all of the invariants. This is the technical property which we need to continue :

*the space of  $G_r$  -invariant polynomials on  $E$  are generated by the homogeneous quadratic invariants* (PROPERTY Q)

A theorem of Weyl [1973] says that this condition does indeed hold for our dual pair.

In our case the dual pair diagram is:

$$u_r^* \longleftarrow H_u \longrightarrow u^*$$

The arrows are the momentum maps  $J_r$  and  $J$  for the respective groups. As usual, we identify the Lie algebras,  $u$ ,  $u_r$  with the vector space of Hermitian operators on the respective spaces. Their dual spaces are identified with Hermitian operators of trace class by using the trace functional. We can write any  $\varphi \in \mathcal{H}_u$  in the form:

$$\varphi = \sum c_{\alpha j} |\psi_{\alpha} \rangle |j \rangle$$

where we used Dirac's notation. Thus  $\{|\psi_{\alpha} \rangle\}$  form a basis for  $H$ ,  $\{|j \rangle\}_{j=1,2,\dots}$  for  $\mathcal{H}_r$ , and  $\{|\psi_{\alpha} \rangle |j \rangle\}$  for  $\mathcal{H}_u$ . We calculate that the images of  $\varphi$  under the two momentum maps are

$$J(\varphi) = \sum_i c_{\alpha i} \bar{c}_{\beta i} |\psi_{\alpha} \rangle \langle \psi_{\beta}|$$

and

$$J_r(\varphi) = \sum_{\alpha} c_{\alpha i} \bar{c}_{\alpha j} |i \rangle \langle j|$$

The formula for  $J(\varphi)$  is exactly the formula (2.4) for a density matrix found in Feynman [1972]

From the formula for J we see that

$$J(\varphi) \geq 0$$

$$\text{trace}(J(\varphi)) = \|\varphi\|^2$$

$$J(\varphi) = 0 \Leftrightarrow \varphi = 0$$

$$\text{rank}(J(\varphi)) = \text{rank}(\varphi)$$

In the last equality we view  $\varphi$  as a linear map  $\mathcal{H}_r \rightarrow \mathcal{H}$ . (Alternatively, rank  $\varphi$  is the minimal number of indecomposable elements,  $\psi \otimes i$ , which make up  $\varphi$ .) It follows that the image of the sphere of normalized states in  $H_u$  consists of the set of density matrices with rank less than or equal to  $k$ , where  $k = \dim \mathcal{H}_r$ . In particular, if  $\dim \mathcal{H}_r \geq (\dim \mathcal{H})$  then every density matrix has the form  $\rho = J(\varphi)$ .

We will now take a density matrix with rank less than or equal to  $k$  and walk through the dual pair construction. First diagonalize  $\rho$  as in equation (II.1a)

$$p = \sum c_i |\psi_i \rangle \langle \psi_i|$$

where  $\psi_i$  forms an orthonormal basis for the image of  $\rho$ . Then set

$$\varphi = \sum \sqrt{c_i} |\psi_i \rangle |i \rangle$$

so that  $J_r(\varphi) = \text{diag}(c_1, c_2, \dots) = \mathbf{c}$ . Here  $\mathcal{H}_u = \mathcal{H} \otimes \mathcal{H}_r \simeq k\mathcal{H} = \mathcal{H} \oplus \dots \oplus \mathcal{H}$  by the isomorphism  $\sum |\varphi(i)\rangle|i\rangle \mapsto (\varphi(1), \varphi(2), \dots)$ . (Note : this map depends on the choice of basis for  $\mathcal{H}_r$  but not for  $\mathcal{H}$ .) Under this isomorphism  $J_r^{-1}(c) = S(c_1, c_2, \dots)$ . Also  $J : J_r^{-1}(c) \rightarrow O = O(\rho)$  is our previous submersion  $\pi : S(c_1, c_2, \dots) \rightarrow O(c_1, c_2, \dots)$ . In summary, the generalized Hopf fibration **is** the canonical reduced space submersion

$$J_r^{-1}(c) \longrightarrow J_r^{-1}(\mathbf{c})/(U_r)_{\mathbf{c}} = M_{\mathbf{c}}$$

Some amusing consequences follow from this last fact. For instance, the problem of finding a “non-Abelian phase formula” is a special case of the general problem of reconstructing the dynamics on a momentum level set given the dynamics on its reduced space.

## II.6. Conclusion: A Flaw and an Oversight

We end the paper by pointing out a flaw and an oversight in our geometrization of quantum statistical mechanics.

*Flaw* : The flaw is that in choosing  $\mathcal{O}$  we have ignored the measurement process. There are two types of measurement processes; those in which no particular value of the measurement is selected, and those in which a particular value is selected from among the possible observed values. The latter are termed “filtering measurement” and the canonical example is the Stern-Gerlach experiment in which an apparatus acts as a spin polarizer. (See, for example, the discussion in Cohen-Tannoudji et al [1977]. ) Upon making the first type of measurement the state  $\rho$  transforms according to

$$\rho \longmapsto \sum \mathbb{P}_i \rho \mathbb{P}_i$$

where  $\{\mathbb{P}_i\}$  is the spectral decomposition of the observable  $A = \sum a_i \mathbb{P}_i$  being measured. In a filtering measurement

$$\rho \longmapsto \mathbb{P}_1 \rho \mathbb{P}_1 / \text{trace}(\mathbb{P}_1 \rho \mathbb{P}_1)$$

where  $a_1$  is the value of the measurement which is selected. I am indebted to Jeeva Anandan for enlightening me as to these two types of measurements and their effects on density matrices.

Either type of measurement will, in general, knock our state out of its co-adjoint orbit  $\mathcal{O}$ . Thus measurements cannot be accounted for by working within a single co-adjoint orbit  $\mathcal{O}$ .

Any state can be achieved by applying some non-filtering measurement to an initial pure state. Thus, to account for these measurements we would have to work on all of  $\mathcal{S}$ . I do not know what the correct geometric structure on  $\mathcal{S}$  is; correct in the sense or correctly reflecting the measurement process. It is almost certainly not Riemannian since it should not be even infinitesimally isotropic: directions along co-adjoint orbits (quantum evolutions) are much different from directions transverse to them and transverse to them (measurements, or wave packet collapses).

For filtering measurements we do not need all of  $\mathcal{S}$ , but rather those matrices  $\rho'$  which can be reached from an initial  $\rho$  by a sequence of filtering measurement. This is some part (perhaps all) of the subvariety of matrices with rank less than or equal to the rank of  $\rho$ .

A series of filtering measurements leads to a series  $\mathcal{O} \rightarrow \mathcal{O}' \rightarrow \mathcal{O}'' \rightarrow \dots$  of co-adjoint orbits. If any of the measurements is non-degenerate (that is, the corresponding eigenvalue is nondegenerate) then the series terminates at  $\mathbb{P}H = \mathcal{S}_{\text{pure}}$ . Different series of filtering measurements lead to different series of orbits. Thus the correct generalization of  $\mathbb{P}H$  might not be a single orbit  $\mathcal{O}$ , but instead a “cascade” of orbits:

$$\begin{array}{ccccc} & & \mathcal{O}' & & \\ & \nearrow & & \searrow & \\ \mathcal{O} & \longrightarrow & \mathcal{O}'' & \longrightarrow & \mathbb{P}H \\ & \searrow & \vdots & \nearrow & \end{array}$$

### Oversight

This is very serious! In our “geometrization” we have completely ignored the most important concepts in statistical mechanics, for example, temperature, entropy, thermal equilibrium, and the Gibbs states. Perhaps some reader will pursue this in the future.

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