Statistical Geometry in Quantum Mechanics

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A statistical model $\mathcal{M}$ is a family of probability distributions, characterised by a set of continuous parameters known as the parameter space. This possesses natural geometrical properties induced by the embedding of the family of probability distributions into the space of all square-integrable functions. More precisely, by consideration of the square-root density function we can regard $\mathcal{M}$ as a submanifold of the unit sphere $\mathcal{S}$ in a real Hilbert space $\mathcal{H}$. Therefore, $\mathcal{H}$ embodies the ‘state space’ of the probability distributions, and the geometry of the given statistical model can be described in terms of the embedding of $\mathcal{M}$ in $\mathcal{S}$. The geometry in question is characterised by a natural Riemannian metric (the Fisher-Rao metric), thus allowing us to formulate the principles of classical statistical inference in a natural geometric setting. In particular, we focus attention on the variance lower bounds for statistical estimation, and establish generalisations of the classical Cramér-Rao and Bhattacharyya inequalities, described in terms of the geometry of the underlying real Hilbert space. As a comprehensive illustration of the utility of the geometric framework, the statistical model $\mathcal{M}$ is then specialised to the case of a submanifold of the state space of a quantum mechanical system. This is pursued by introducing a compatible complex structure on the underlying real Hilbert space, which allows the operations of ordinary quantum mechanics to be reinterpreted in the language of real Hilbert space geometry. The application of generalised variance bounds in the case of quantum statistical estimation leads to a set of higher order corrections to the Heisenberg uncertainty relations for canonically conjugate observables.

1. Introduction

The purpose of this paper is twofold: first, to develop a concise geometric formulation of statistical estimation theory; and second, the application of this formalism to quantum statistical inference. Our intention is to establish the basic concepts of statistical estimation within the framework of Hilbert space geometry. This line of enquiry, although suggested by Bhattacharyya (1942), Rao (1945), and Dawid (1975,1977), has not hitherto been pursued in the spirit of the fully geometric program that we undertake here. In 1945 Rao introduced a Riemannian metric, in local coordinates given by the components of the Fisher information matrix, on the parameter space of a family of probability distributions. He also introduced the corresponding Levi-Civita connection associated with the Fisher
information matrix, and proposed the geodesic distance induced by the metric as a measure of dissimilarity between probability distributions. Thirty years after Rao’s initial work, Efron (1975) carried the argument a step forward when he introduced, in effect, a new affine connection on the parameter space manifold, and thus shed light on the role of the embedding curvature of the statistical model in the relevant space of probability distributions. The work of Efron has been followed up and extended by a number of authors (see, e.g., Amari 1982, 1985, Barndorff-Nielsen, Cox, and Reid 1986, and Kass 1989), particularly in the direction of asymptotic inference. However, the applicability of modern differential geometric methods to statistics remains in many respects a surprising development, about which there is still much to be learned.

In a remark on Efron’s construction, Dawid (1975) asked whether there might be a fundamental role played by the Levi-Civita connection in statistical analysis. The aim of this paper in part is to answer this important question, by studying statistical inference from a Hilbert space perspective. In particular, we shall study the geometric properties of a statistical model $\mathcal{M}$ induced when we embed $\mathcal{M}$ via the square-root map in the unit sphere $S$ in a real Hilbert space $H$. This leads in a natural way to the Levi-Civita connection on $\mathcal{M}$.

It was also pointed out by Dawid (1977), in the case of an embedding given by the square-root of the likelihood function, that the Hilbert space norm induces a spherical geometry (see also Burbea 1986). If the density function is parameterised by a set of parameters $\theta$, then for each value of $\theta$ we have a corresponding point on the unit sphere $S$ in the Hilbert space $H$. By choosing a basis in $H$, we can associate a unit vector $\xi^a(\theta)$ with this point, and work with the abstract vector $\xi^a(\theta)$ instead of $\sqrt{p_\theta(x)}$. The index ‘$a$’ is abstract in the sense that we do not necessarily regard it as ‘taking values’; instead, it serves as a kind of ‘place-keeper’ for various tensorial operations. We show how the abstract index approach can be used as a powerful tool in statistical investigations.

Our program includes the exploitation of this methodology to study geometrical and statistical aspects of quantum mechanics. The specialisation to quantum theory requires an extra ingredient, namely, a complex structure. Thus, if we take our real Hilbert space and impose on it a complex structure, compatible with the real Hilbert space metric, the resulting geometry is sufficiently rich to allow us to introduce all of the standard operations of quantum theory.

While the conventional approach to quantum statistical estimation has essentially been merely ‘by analogy’ with classical estimation, our approach differs in the sense that we view quantum estimation theory as arising in essence as a natural extension of the classical theory, when the theory is ‘enriched’ with the addition of a complex structure, and the system of random variables is expanded to include incompatible observables.

By way of contrast we note that most of the current literature of quantum statistical estimation (see, e.g., Accardi and Watson 1994, Braunstein and Caves 1994, Brody and Meister 1996a,b, Helstrom 1976, Holevo 1982, Ingarden 1981, Jones 1994, Malley and Hornstein 1993, Nagaoka 1994, and references cited therein) takes the space of density matrices as the relevant state space in terms of which estimation problems are formulated, the view there being that the ‘space of density matrices’ is the quantum mechanical analogue of the ‘space of density functions’ when we consider the quantum estimation problem.
In our approach, however, we find it useful to emphasise the role of the space of pure quantum states. In fact, the space of density matrices has a very complicated geometric structure, owing essentially to the various levels of ‘degeneracy’ a density matrix can possess, and the relation of these levels to one another. It can be argued that to tackle the quantum estimation problem head-on from a density matrix approach is not necessarily advantageous. In any case, the consideration of pure states allows us to single out most sharply the relation between classical statistical theory and quantum statistical theory, and in such a way that the geometry takes on a satisfactory character. The extension of our approach to general states will be taken up elsewhere.

The plan of the paper is as follows. In §2, the geometry of the parameter space induced by the Hilbert space norm is introduced by means of an index notation. This notation is employed here partially for the purpose of simplifying complicated calculations, and its usefulness in this respect will become evident. The index notation also greatly facilitates the geometrical interpretation of the operations being represented here. Attention is drawn to formula (2.5) for the Riemannian metric on $\mathcal{M}$, and the argument given in Proposition 2 that indicates the special status of the Levi-Civita connection. Our idea is to reformulate a number of the standard concepts of statistics in the language of Hilbert space geometry. In particular, in §§3 and §4 we develop the theory of the maximum likelihood estimator (MLE) and the Cramér-Rao (CR) variance lower bound, for which novel geometrical interpretations are provided. See, for example, Proposition 4 and Theorem 1. Also, note Proposition 6 where a striking link is made between an essentially statistical quantity and an essentially geometric quantity.

In §4 we consider in some detail properties of the canonical family of exponential distributions, which can be described concisely in terms of the Hilbert space geometry. This material also has interesting applications to statistical mechanics and thermal physics, which we discuss elsewhere.

In §5, a set of higher-order corrections to the CR lower bound is obtained, leading to what might appropriately be called generalised Bhattacharyya bounds, given in Proposition 8. However, unlike the original Bhattacharyya bound, the new variance bounds generally depend upon features of the estimator. Nevertheless, in certain cases of interest the result is independent of the specific choice of estimator. This will be illustrated with examples from problems in quantum estimation. A brief account of multi-parameter situation is given in §6.

After some comments on the transition from classical to quantum theory in §7, a general geometric formulation of ordinary quantum mechanics is developed in §§8 and §9 in terms of a real Hilbert space setting. In §§10 and §11 we apply our geometric estimation theory to the quantum mechanical state space. We are interested, in particular, in the variance bounds associated with pairs of canonically conjugate observables. Here we study in detail the example of time estimation in quantum theory. This is pursued by means of a nonorthogonal resolution of unity, known as a probability operator-valued measure (POM), which allows us to construct a well defined maximally symmetric time ‘observable’ within the framework of ordinary quantum mechanics. Finally in §12, we apply the generalised variance lower bounds to obtain a remarkable set of higher order corrections to the Heisenberg relations.
2. Index Notation and Fisherian Geometry

Consider a real Hilbert space \( \mathcal{H} \), equipped with a symmetric inner product which we denote \( g_{ab} \). As noted above, we adopt an index notation for Hilbert space operations. Let us write \( \xi^a \) for a typical vector in \( \mathcal{H} \). If \( \mathcal{H} \) is finite, the index can be thought of as ranging over a set of integers, while in the infinite dimensional case, the index is 'abstract'. See Geroch (1971a,b), Penrose and Rindler (1984, 1986), or Wald (1994) for further details of this notation. Our intention here is not to present a rigorous account of the matter, which would be beyond the scope of the present work, but rather to illustrate the utility of the index calculus by way of a number of examples. In particular, in the infinite dimensional case there are technical conditions concerning the domains of operators that require care—these will not concern us here in the first instance, though in our treatment of quantum estimation more attention will be paid in this respect.

Suppose we consider the space of all probability density functions \( p(x) \) on the sample space \( \mathbb{R}^n \). By taking a square root we can map each density function to a point on the unit sphere \( S \) in \( \mathcal{H} = L^2(\mathbb{R}^n) \), given by \( g_{ab} \xi^a \xi^b = 1 \). A random variable in \( \mathcal{H} \) is then represented by a symmetric bilinear form, e.g., \( X_{ab} \), with expectation \( X_{ab} \xi^a \xi^b \) in the state \( \xi^a \), that is,

\[
E_{\xi}[X] = X_{ab} \xi^a \xi^b .
\]

(2.1)

In terms of the conventional statistical notation, we can associate \( \xi^a \) with \( p(x)^{1/2} \), \( X_{ab} \) with \( x \delta(x - y) \), and hence \( X_{ab} \xi^a \xi^b \) with the integral

\[
\int_x \int_y x \delta(x - y)p(x)^{1/2}p(y)^{1/2}dxdy ,
\]

(2.2)

which reduces to the expectation. This line of reasoning can be extended to more general expressions. Thus, for example, \( X_{ab} X_{cd} \xi^a \xi^c \) is the expectation of the square of the random variable \( X_{ab} \), and the variance of \( X_{ab} \) in the state \( \xi^a \) is

\[
\text{Var}_{\xi}[X] = \tilde{X}_{ac} \tilde{X}^c_{b} \xi^a \xi^b ,
\]

(2.3)

where \( \tilde{X}_{ab} = X_{ab} - g_{ab}(X_{cd} \xi^c \xi^d) \) represents the deviation \( \Delta X \) of the random variable from its mean. Likewise for the covariance of the random variables \( X_{ab} \) and \( Y_{ab} \) in the state \( \xi^a \) we can write

\[
\text{Cov}_{\xi}[X,Y] = \tilde{X}_{ac} \tilde{Y}^c_{b} \xi^a \xi^b .
\]

(2.4)

Note that if \( \xi^a \) is not normalised, then the formulae above can be generalised with the inclusion of suitable normalisation factors.

We consider now the unit sphere \( S \) in \( \mathcal{H} \), and within this sphere a submanifold \( \mathcal{M} \) given parametrically by \( \xi^a(\theta) \), where \( \theta^i (i = 1, \cdots, r) \) are local parameters. We write \( \partial_i \) for \( \partial / \partial \theta^i \).

**Proposition 1.** (Fisher-Rao metric). In local coordinates, the Riemannian metric \( G_{ij} \) on \( \mathcal{M} \), induced by \( g_{ab} \), given by

\[
G_{ij} = 4g_{ab} \partial_i \xi^a \partial_j \xi^b ,
\]

(2.5)

is the Fisher information matrix.

The proof is as follows. We note that the squared distance between the endpoints of two vectors \( \xi^a \) and \( \eta^a \) in \( \mathcal{H} \) is \( D^2 = g_{ab}(\xi^a - \eta^a)(\xi^b - \eta^b) \). If both
endpoints lie on $\mathcal{M}$, and $\eta^a$ is obtained by infinitesimally displacing $\xi^a$ in $\mathcal{M}$, i.e.,

$$\eta^a = \xi^a + \partial_i \xi^a d\theta^i,$$

then the separation $ds$ between the two endpoints on $\mathcal{M}$ is

$$ds^2 = \frac{1}{4} G_{ij} d\theta^i d\theta^j,$$  \hspace{1cm} (2.6)

where $G_{ij}$ is given as in (2.3). The factor of $\frac{1}{4}$ arises from the conventional definition of the Fisher information matrix in terms of the log-likelihood function $l(x|\theta) = \ln p(x|\theta)$, given by

$$G_{ij} = \int_x p(x|\theta) \partial_i l(x|\theta) \partial_j l(x|\theta) dx.$$  \hspace{1cm} (2.7)

By differentiating $g_{ab} \xi^a \xi^b = 1$ twice, we obtain an alternative expression for $G_{ij}$, that is, $G_{ij} = -4 \xi_a \partial_i \partial_j \xi^a$. This formula turns out to be useful in statistical mechanics (see, e.g., Brody and Rivier 1995, Streater 1996), where the geometry of the relevant coupling constant space can be investigated. The induced geometry of $\mathcal{M}$ can be studied in terms of the metric $G_{ij}$ and our subsequent analysis will be pursued on this basis. To start, we note the following result:

**Lemma 1.** The Christoffel symbols for the metric connection arising from $\mathcal{G}$ are given by $\Gamma^i_{jk} = 4 G^{il} \partial_j \xi^l \partial_k \xi_a$.

This can be obtained by insertion of (2.3) into the familiar formula

$$\Gamma^i_{jk} = \frac{1}{2} G^{il} (\partial_j G_{kl} + \partial_k G_{jl} - \partial_l G_{jk})$$  \hspace{1cm} (2.8)

for the Levi-Civita (metric) connection. Now, let $\nabla_i$ denote the standard Levi-Civita covariant derivative operator associated with $G_{ij}$, for which $\nabla_i G_{jk} = 0$ and $\nabla_i$ is torsion free. Then a straightforward calculation shows that

$$G_{ij} = -4 \xi_a \nabla_i \nabla_j \xi^a.$$  \hspace{1cm} (2.9)

A question that naturally arises is, are there any other ‘natural’ connections associated with the given Hilbert space structure? This requires one to construct a tensor of the form $Q_{ijk}$ purely from the metric and covariant derivatives of the state vector $\xi^a$. The answer to this question is of relevance, since we would like to know whether it is possible to construct a set of affine connections (e.g., Amari’s $\alpha$-connection) purely in terms of the given basic Hilbert space geometry, or whether extra structure is required. Clearly, the only possibilities are $\nabla_i \xi^a \nabla_j \nabla_k \xi_a$ and $\xi^a \nabla_i \nabla_j \nabla_k \xi_a$. However, some straightforward algebra leads us to the following result:

**Proposition 2.** The expressions $\nabla_i \xi^a \nabla_j \nabla_k \xi_a$ and $\xi^a \nabla_i \nabla_j \nabla_k \xi_a$ vanish. Thus, no natural three-index tensors can be constructed in Hilbert space, and the Levi-Civita connection is distinguished amongst possible $\alpha$-connections.

The proof is as follows. First, note that $\nabla_k G_{ij} = 0$ implies $\nabla_k (\nabla_i \xi^a \nabla_j \xi_a) = 0$, and hence $\nabla_k \nabla_i \xi^a \nabla_j \xi_a + \nabla_k \nabla_j \xi^a \nabla_i \xi_a = 0$. On the other hand, it follows from (2.9), by differentiation, that $\nabla_k \xi_a \nabla_i \nabla_j \xi_a = -\xi_a \nabla_k \nabla_i \nabla_j \xi_a$. Therefore, we deduce that $\nabla_k \nabla_i \xi^a \nabla_j \xi_a = \xi_a \nabla_i \nabla_j \nabla_k \xi^a$, and that $\xi_a \nabla_i \nabla_j \nabla_k \xi_a = 0$. Since $\xi_a \nabla_i \nabla_j \nabla_k \xi^a$ is antisymmetric over the indices $i, j$, it follows that

$$\xi_a \nabla_i \nabla_j \nabla_k \xi^a = \frac{1}{2} \xi_a R_{ijk} \nabla_l \xi^a$$  \hspace{1cm} (2.10)
where $R_{ijk}^l$ is the Riemann tensor, defined by $(\nabla_i \nabla_j - \nabla_j \nabla_i)V_k = R_{ijk}^lV^l$ for any smooth vector field $V_k$. However, $\xi_a \nabla_i \xi^a$ vanishes in (2.10), since $\xi^a \xi_a = 1$, and that establishes the desired result.

Therefore, to introduce other affine connections on $\mathcal{M}$, such as Amari’s $\alpha$-connection, additional structure on the given Hilbert space is required. Although these ‘artificial’ connections are useful in certain statistical inference problems, such as higher order asymptotics, we conclude that from a Hilbert space point of view the Levi-Civita connection is the only ‘natural’ connection associated with the space of probability measures.

Note, incidentally, that in the case of a one-parameter family of distributions, the Fisher information is given by $G = 4g_{ab}\dot{\xi}^a \dot{\xi}^b$, where the dot denotes differentiation with respect to $\theta$. Thus, the Fisher information is related in a simple way to the ‘velocity’ along the given curve in Hilbert space. This is a result that, as we see later (cf. Proposition 10), has profound links with an analogous construction in quantum mechanics (Anandan and Aharonov 1990).

3. Maximum Likelihood Estimation

Suppose we are given a random variable $X_{ab}$ which takes real values, and told that the result of a sampling of $X_{ab}$ is the number $x$. We are interested in a situation where we have a one-parameter family of normalised states $\xi^a(\theta)$ characterising the distribution of $x$. The parameter $\theta$ determines the unknown state of nature, and we wish to estimate $\theta$ by use of maximum likelihood methods; that is, we wish to associate with a given value of $x$ an appropriate value of $\theta$ that maximises the likelihood function. In this section, we present a geometrical characterisation of the maximum likelihood estimator (MLE), which has an elegant Hilbert space interpretation once we single out a ‘preferred’ random variable $X_{ab}$.

**Proposition 3.** Given the random variable $X_{ab}$, the normalised state vector $\xi^a(\theta)$, and the measurement outcome $x$, the parameterised likelihood function $p(x|\theta)$ is given by

$$p(x|\theta) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \xi^a \xi_b \exp \left[ i\lambda(X_b^a - x\delta_b^a) \right] d\lambda .$$

(3.1)

This can be seen as follows. We define the projection operator $\Delta^a_b(X, x)$ associated with the random variable $X_{ab}$ and the measurement outcome $x$ by

$$\Delta^a_b(X, x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp \left[ i\lambda(X_b^a - x\delta_b^a) \right] d\lambda .$$

(3.2)

We note that $\Delta^a_b(X, x)\Delta^b_c(X, y) = \delta^a_c \delta(x - y)$, and that $X_{ab}$ can be recovered from $\Delta_{ab}(X, x)$ via the spectral resolution

$$X_{ab} = \int_{-\infty}^{\infty} x \Delta_{ab}(X, x) dx .$$

(3.3)

Then, the likelihood function $p(x|\theta)$ is the expectation of $\Delta_{ab}$ in the state $\xi^a$, i.e.,

$$p(x|\theta) = \Delta_{ab} \xi^a \xi^b .$$

(3.4)

Alternatively, $p(x|\theta)$ can be obtained by taking the Fourier transform of the
characteristic function
\[ \phi_\theta(\lambda) = \xi^a \xi_b \exp \left[ i \lambda X_a^b \right], \quad (3.5) \]
which leads back to (3.1). The maximum likelihood estimate \( \bar{\theta}(x) \) for \( \theta \), assuming it exists and is unique, is obtained by solving
\[ \Delta_{ab}(X, x) \xi^a \xi^b |_{\theta = \bar{\theta}} = 0. \quad (3.6) \]
Geometrically, this means that, along the curve \( \xi^a(\theta) \) on the sphere \( \mathcal{S} \), \( \bar{\theta}(x) \) maximises the quadratic form \( \Delta_{ab} \xi^a \xi^b \). Conversely, if \( \bar{\theta}(x) \) is the MLE for the parameter \( \theta \), then the corresponding random variable in \( \mathcal{H} \) is
\[ \Theta_{ab}(X) = \int_{-\infty}^{\infty} \bar{\theta}(x) \Delta_{ab}(X, x) dx. \quad (3.7) \]
If we let \( \Delta_x(\xi^a) \) denote the quadratic form \( \Delta_{ab} \xi^a \xi^b \) on \( \mathcal{H} \), then equation (3.3) for the MLE can be rewritten as \( \xi^a \nabla_a \Delta_x = 0 \), where the ‘gradient’ operator \( \nabla_a \) is defined by \( \nabla_a = \partial / \partial \xi^a \), so \( \nabla_a(\Delta_{bc} \xi^b \xi^c) = 2 \Delta_{ab} \xi^b \). Thus, for each given value of \( x \) we can foliate \( \mathcal{S} \) with hypersurfaces of constant \( \Delta_x \). This leads us to the following characterisation of the MLE.

**Proposition 4.** The maximum likelihood estimate \( \bar{\theta}(x) \) is the value of \( \theta \), for each given value of \( x \), such that the tangent of the curve \( \xi^a(\theta) \) is orthogonal to the normal vector of the constant \( \Delta_x \) surface passing through the point \( \xi^a(\theta) \).

Thus, we see that maximum likelihood estimation has a characterisation in terms of Hilbert space geometry that can be achieved by introducing extra structure on \( \mathcal{H} \), namely, by ‘singling out’ a particular observable. This is natural in the context of some classical statistical investigations, though for quantum statistical inference we may wish to avoid the introduction of ‘preferred’ observables.

4. *Cramér-Rao Lower Bound and Exponential Families*

In the case of a general estimation problem, a lower bound can be established for the variance with which the estimate deviates from the true value of the relevant parameter. Our intention in this section is to present a geometric characterisation of this bound. In doing so we also make some observations about the geometry of exponential families of distributions, of relevance to statistical physics. Consider a curve \( \xi^a(\theta) \) in \( \mathcal{S} \). We say that a random variable \( T_{ab} \) is an *unbiased estimator* for the function \( \tau(\theta) \) if
\[ T_{ab} \xi^a(\theta) \xi^b(\theta) = \tau(\theta). \quad (4.1) \]
For convenience, we define a mean-adjusted deviation operator \( \bar{T}_{ab} T_{ab} \equiv T_{ab} - \tau g_{ab} \). Note that \( \bar{T}_{ab} \xi^a \xi^b = 0 \), and that the variance of \( T \) is given by \( \text{Var}_x[T] = \bar{T}_{ab} T_{ab} \xi^a \xi^c \).

Since \( T_{ab} \xi^a \xi^b = \tau \), we obtain \( 2T_{ab} \xi^a \xi^b = \tau \), hence \( 2\bar{T}_{ab} \xi^a \xi^b = \tau \). Therefore, if we define \( \eta_b = \bar{T}_{ab} \xi^b \), we have \( \eta_b \xi^b = \bar{T}_{ab} \xi^a \xi^b \). Hence by use of the Cauchy-Schwarz inequality \( (\eta^a \eta_a)(\xi^a \xi_a) \geq (\eta_a \xi_a)^2 \), we are led to the following result.

**Theorem 1.** (Cramér-Rao inequality). Let \( T \) be an unbiased estimator for a function \( \tau(\theta) \) where \( \theta \) parametrises a one-dimensional family of states \( \xi^a(\theta) \) in

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$S \in \mathcal{H}$. Then, the variance lower bound in the state $\xi^a$ is given by

$$\text{Var}_\xi[T] \geq \frac{\dot{T}^2}{4\xi^a \dot{\xi}^a}. \quad (4.2)$$

It is clear from the preceding argument that the CR lower bound is attained only if $\dot{\xi}^a = c\eta^a$ for some constant $c$, which by rescaling $\theta$ we can set to $1/2$ without loss of generality. Thus, for any curve $\xi^a(\theta)$ achieving the lower bound, we obtain the differential equation

$$\dot{\xi}^a = \frac{1}{2} T^a_b \xi^b, \quad (4.3)$$

The solution of (4.3) is the canonical exponential family of distributions, given by the following elegant formula:

$$\xi^a(\theta) = \exp\left(\frac{1}{2} \theta T^a_b \xi^b\right) \frac{\sqrt{\exp[\theta T^a_b \xi^b]}}{q^a q^b}, \quad (4.4)$$

where the normalised state vector $\xi^a(0) = q^a / (q_b q^b)^{1/2}$ determines a prescribed initial distribution. Without loss of generality we can set $q_a q^a = 1$. This expression leads us to an interesting geometrical interpretation of the exponential family. We consider the unit sphere $S$ in $\mathcal{H}$, with the standard spherical geometry induced on it by $g_{ab}$. Let

$$\tau = \frac{T_{ab} \xi^b}{g_{cd} \xi^c \xi^d} \quad (4.5)$$

be a quadratic form defined on $S$. Then $S$ can be foliated by surfaces of constant $\tau$. Since according to (4.3) the tangent vector $\dot{\xi}^a$ is parallel to the gradient of the function $\tau(\xi^a)$, we conclude that:

**Proposition 5.** The canonical exponential family of distributions $\xi^a(\theta)$, with initial distribution $q^a$, is given by the unique curve through the point $q^a$ that is everywhere orthogonal to the family of foliating $\tau$-surfaces.

In particular, as we show in Proposition 6 below, the variance $\text{Var}_\xi[T]$ at the point $\xi^a$ is a quarter of the squared magnitude of the gradient of the surface through $\xi^a$, given by $\nabla_a \tau$. The Fisher information, on the other hand, is four times the squared magnitude of the tangent vector to the curve at $\xi^a$. Since the inner product of the tangent vector $\xi^a$ and the normal vector $\nabla_a \tau$ is the derivative $\dot{\tau}$, it follows that $\text{Var}_\xi[T] \geq \dot{\tau}^2 / \mathcal{G}$, the CR inequality.

**Proposition 6.** Let $\nabla_a = \partial / \partial \xi^a$ denote the gradient operator in $\mathcal{H}$. Then the variance of an unbiased estimator $T_{ab}$ for a function $\tau$ in the state $\xi^a$ is given, on the sphere $S$, by

$$\text{Var}_\xi[T] = \frac{1}{4} \nabla_a \tau \nabla^a \tau. \quad (4.6)$$

This can be verified as follows. By definition, we have a quadratic form $\mathcal{F}$.
on $\mathcal{H}$. Then, by differentiation, we obtain

$$
\nabla_a \tau = \frac{2T_{ab}\xi^b}{\xi^c\xi_c} - \frac{2(T_{bc}\xi^b_\xi^c)\xi_a}{(\xi^d\xi_d)^2},
$$

(4.7)

from which it follows that

$$
\frac{1}{4} \nabla_a \nabla_a \tau = \frac{(T_{ac}T^c_b - \tau^2 g_{ab})\xi^a_\xi^b}{(\xi^c\xi_c)^2}.
$$

(4.8)

Since the variance of $T_{ab}$ is given by $\text{Var}_a[T] = (T_{ac}T^c_b - \tau^2 g_{ab})\xi^a_\xi^b / (\xi^c\xi_c)^2$, equation (4.8) follows at once after we restrict (13) to the sphere $\xi^a\xi_a = 1$.

In the case of the exponential family of distributions, the corresponding density function is given by $p(x|\theta) = q(x) \exp[x\theta - \psi(\theta)]$, where $q(x)$ is the prescribed initial density, and the normalisation constant $\psi(\theta)$ is given by

$$
\psi(\theta) = \ln \int_{-\infty}^{\infty} e^{x\theta} q(x) dx = \ln \left( \exp[\theta T_a q^a q^b] \right).
$$

(4.9)

It is interesting to note that the log-likelihood $l(x|\theta)$ for an exponential family has a natural geometric characterisation in $\mathcal{H}$. Suppose we consider a multi-parameter exponential distribution given by

$$
\xi^a(\theta) = \exp \left[ \frac{1}{2} \sum_{j=1}^{r} \theta^j T_{(j) b} - \psi(\theta) \delta^a_b \right] q^b
$$

(4.10)

Our idea is to construct a random variable $l_{ab}$ in $\mathcal{H}$ that represents the log-likelihood $l(x|\theta)$ for this family of distributions. We define the log-likelihood $l^a_b$ associated with an exponential family of distributions by the symmetric operator

$$
l^a_b(\theta) = \sum_{j=1}^{r} \theta^j T_{(j) b} - \psi(\theta) \delta^a_b.
$$

(4.11)

Note that the expectation of $l_{ab}$ gives the Shannon entropy, that is,

$$
S_{\xi}(\theta) = l_{ab} \xi^a \xi^b = \sum_{j=1}^{r} \theta^j \tau_{(j)}(\theta) - \psi(\theta).
$$

(4.12)

The second expression is the familiar one for the Legendre transformation that relates the entropy $S(\theta)$ to the normalisation constant $\psi(\theta)$. In the case of a one-parameter family of exponential distributions, the gradient $\nabla_a \tau$ can be written $\frac{1}{2} \nabla_a \tau = \tilde{l}_{ab} \xi^b$. In the multi-parameter case this becomes $\frac{1}{2} \nabla_a \tau_{(j)} = \xi^b \partial_j l_{ab}$, which leads to the following formula for the Fisher information:

**Proposition 7.** The Fisher information matrix $G_{ij}$ can be expressed in terms of the log-likelihood $l^a_b$ by the formula $G_{ij} = \partial_i l_{ac} \partial_j l^c_b \xi^a_\xi^b$.

Thus in the case of an exponential family of distributions we find the Fisher-Rao metric is given by the covariance matrix of the estimators $\tilde{T}_{(i)}$:

$$
G_{ij} = (T_{(i) ac} - \partial_i \psi \delta_{ac}) (T_{(j) b}^c - \partial_j \psi \delta_{bc}) \xi^a_\xi^b \equiv E_{\xi} \left[ \tilde{T}_{(i)} \tilde{T}_{(j)} \right].
$$

(4.13)
5. Generalised Bhattacharyya Bounds

We have observed that the exponential family is the only family capable of achieving the variance lower bound, providing we choose the right function $\tau(\theta)$ of the parameter to estimate. For other families of distributions, the variance exceeds the lower bound. In order to obtain sharper bounds in the general situation, we consider the possibility of establishing higher-order corrections to the CR lower bound. Our approach is related to that of Bhattacharyya (1946, 1947, 1948). However, in a Hilbert space context, we are led along a different route from Bhattacharyya’s original considerations, since in his approach the likelihood function $p(x; \theta)$ plays a crucial role. First, we shall formulate a new, Bhattacharyya-style derivation of the CR inequality. We note that if $T_{ab}$ is an unbiased estimator for the function $\tau(\theta)$, then so is $R_{ab} = T_{ab} + \lambda \xi(a) \xi(b)$, for an arbitrary constant $\lambda$. We choose the value of $\lambda$ that minimises the variance of $R_{ab}$. This implies $\lambda = -\dot{\tau}/2 \xi^a \xi_a$, and hence

$$\min (\text{Var}_\xi [R]) = \text{Var}_\xi [T] - \frac{\dot{\tau}^2}{4 \xi^a \xi_a}. \quad (5.1)$$

Since $\text{Var}_\xi [R] \geq 0$, we are immediately led back to the CR inequality \[5.2\].

Now we try to improve on this by incorporating terms with higher-order derivatives. Let us denote the $r$-th derivative of $\xi^a$ with respect to the parameter $\theta$ by $\xi^{(r)a} = d^r \xi^a / d\theta^r$. We write $\xi^{(r)a}_\parallel$ for the projection of $\xi^{(r)a}$ orthogonal to $\xi^a$ and to all the lower order derivatives, so $\xi^{(r)a}_\parallel \xi^a = 0$ and $\xi^{(r)a}_\parallel \xi^{(s)a} = 0$ for $s < r$. If $T_{ab}$ is an unbiased estimator for $\tau(\theta)$, so is the symmetric tensor $R_{ab}$ defined by

$$R_{ab} = T_{ab} + \sum_r \lambda_r \xi(a) \xi^{(r)b}_\parallel \quad (5.2)$$

for arbitrary constants $\lambda_r$. We only consider values of $r$ such that $\xi^{(r)} \neq 0$, assuming that the relevant derivatives exist and are linearly independent. A straightforward calculation leads us to the values of $\lambda_r$ minimising the variance of $R$, and we obtain

$$\min (\text{Var}_\xi [R]) = \text{Var}_\xi [T] - \sum_r \frac{(T_{ab} \xi^a \xi^{(r)b}_\parallel)^2}{g_{ab} \xi^{(r)a} \xi^{(r)b}}. \quad (5.3)$$

Since $\text{Var}_\xi [R]$ is nonnegative, we thus deduce the following generalised Bhattacharyya bounds for the variance of the estimator:

$$\text{Var}_\xi [T] \geq \sum_r \frac{(T_{ab} \xi^a \xi^{(r)b}_\parallel)^2}{g_{ab} \xi^{(r)a} \xi^{(r)b}}. \quad (5.4)$$

This derivation is ‘historical’ in flavour in the sense that it parallels certain aspects of the original argument of Bhattacharyya. However, Proposition 3 allows us to reexpress \[5.3\] in the form of a simple geometric inequality. That is, given the gradient vector $\nabla_\theta \tau$ in $\mathcal{H}$, the squared length of this vector is not less than the sum of the squares of any of its orthogonal components with respect to a suitable basis. To this end, we consider the vectors based on the state $\xi^a$ and its higher order derivatives, and form the orthonormal vectors given by $\xi^{(r)a} / (\xi^{(r)a} \xi^{(r)b} \xi^{(r)b}_\parallel)^{1/2}$. It follows from the basic relation \[5.4\] deduced in Proposition 6 that:

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Proposition 8. The generalised variance lower bounds for an unbiased estimator $T$ of a function $\tau$ can be expressed in the form:

$$\text{Var}_\xi[T] \geq \frac{1}{4} \sum_r \frac{\left(\xi^{(r)} a \nabla_a \tau\right)^2}{\left(\xi^{(r)} b \xi^{(r)} b\right)}.$$  \hspace{1cm} (5.5)

Clearly for $r = 1$ we recover the CR inequality. Unlike the classical Bhat-tacharyya bounds, the generalised bounds are not necessarily independent of the estimator $T$. In our applications to quantum mechanics, however, we shall indicate some important examples of higher-order bounds that are indeed independent of the specific choice of estimator. See Brody and Hughston (1996d) for a related example drawn from classical thermal physics where the bounds are also systematically independent of the estimator.

We remark, incidentally, that the denominator terms in equation (5.5) give rise to natural geometric invariants. For example, in the case $r = 2$ we have

$$\hat{\xi}^{(2)} a \hat{\xi}^{(2)} b = (\dot{\xi}^a \xi^b g_{ab})^2 K^2_{\xi},$$  \hspace{1cm} (5.6)

where $K^2_{\xi}$ is the curvature of the curve $\xi^a(\theta)$ in $S$. In particular, we obtain

Lemma 2. In the case of the canonical exponential family of distributions, specified in equation (4.4), the curvature of $\xi^a(\theta)$ is given by:

$$K^2_{\xi} = \frac{\langle \dot{T}^4 \rangle}{\langle T^2 \rangle^2} - \frac{\langle \dot{T}^3 \rangle^2}{\langle T^2 \rangle^3} - 1.$$  \hspace{1cm} (5.7)

As a matter of interpretation we note that the first term in the right hand side of (5.7) is the kurtosis (measure of sharpness) of the distribution, while the second term is the skewness (measure of asymmetry). A classical statistical inequality relating these quantities (cf. Stuart and Ord 1994) ensures that $K^2_{\xi} \geq 0$. In the case of the exponential family we have $\dot{\xi}^{(2)} a \nabla_a \tau = 0$, i.e., the ‘acceleration vector’ $\dot{\xi}^{(2)} a$ lies in the tangent space of the surfaces generated by constant values of the estimator function $\tau(\theta)$.

6. Multiple Parameters

The geometrical constructions so far considered are based mainly upon one-parameter families of distributions. However, for completeness here we sketch some useful results applicable to multi-parameter distributions. First, consider the case where we estimate a single function $\tau(\theta)$ depending upon several parameters $\theta^i$. A straightforward argument shows that the CR inequality then takes the form

$$\text{Var}_\xi[T] \geq \sum_{ij} G^{ij} \tau_i \tau_j,$$  \hspace{1cm} (6.1)

where $\tau_i = \partial_i \tau(\theta)$ and $G^{ij}$ is the inverse of the Fisher information matrix. In a more general situation, we might have several estimators $T_{(\alpha)ab}$ ($\alpha = 1, \cdots, n$) labelled by an index $\alpha$, with $T_{(\alpha)ab} \xi^a \xi^b = \tau_{\alpha}(\theta)$. For an arbitrary set of constants $\Lambda_\alpha$, we form the sums $T_{ab} = \sum_\alpha \Lambda_\alpha T_{(\alpha)ab}$ and $\tau(\theta) = \sum_\alpha \Lambda_\alpha \tau_{\alpha}$. It follows that...
the CR inequality (6.1) holds for the summed expressions $T_{ab}$ and $\tau(\theta)$. However, since $\Lambda_\alpha$ is constant, the variance of $T$ can be written

$$\text{Var}_\xi[T] = \sum_{\alpha\beta} C_{\alpha\beta} \Lambda_\alpha \Lambda_\beta,$$

(6.2)

where $C_{\alpha\beta} = \text{Cov}_\xi[T_\alpha, T_\beta]$ is the covariance matrix for the estimators $T_\alpha$. Therefore, the CR inequality can be rewritten in the form

$$\sum_{\alpha\beta} \text{Cov}_\xi[T_\alpha, T_\beta] \Lambda_\alpha \Lambda_\beta - \sum_{\alpha\beta} G_{ij} \partial_i \tau_\alpha \partial_j \tau_\beta \Lambda_\alpha \Lambda_\beta \geq 0.$$  (6.3)

Since this holds for arbitrary values of $\Lambda_\alpha$, we obtain the following matrix inequality for the covariance lower bound.

**Proposition 9.** Let $T_\alpha$ ($\alpha = 1, 2, \cdots, r$) be unbiased estimators for the functions $\tau_\alpha(\theta)$. The lower bound for the covariance matrix is given by

$$\text{Cov}_\xi[T_\alpha, T_\beta] \geq G_{ij} \partial_i \tau_\alpha \partial_j \tau_\beta.$$  (6.4)

This equation is to be interpreted in the sense of saying that the difference between the left and right hand sides is nonnegative definite.

### 7. From Classical to Quantum Theory

In the foregoing material, we have reformulated various aspects of parametric statistical inference in terms of the geometry of a real Hilbert space. In particular, the abstract index notation has enabled us very efficiently to obtain results relating to statistical curvatures and variance lower bounds. One of the main reasons we are interested in formulating statistical estimation theory in a Hilbert space framework is on account of the connection with quantum mechanics, which becomes more direct when pursued in this manner, thus enabling us in many respects to unify our view of classical and quantum statistical estimation.

The fact that in our approach to classical statistical estimation the geometry in question is a Hilbert space geometry is a result that physicists may find surprising. This is because the general view in physics is that the Hilbert space structure associated with the space of states in nature is special to quantum theory, and has no analogue in classical probability theory and statistics. We have seen, however, that a number of structures already present in the classical theory are highly analogous to associated quantum mechanical structures; but the correspondence is only readily apparent when the classical theory is reformulated in the appropriate geometrical framework. A key point is that if we supplement the real Hilbert space $\mathcal{H}$ with a *compatible complex structure*, then this paves the way for a natural attack on problems of quantum statistical inference, and it becomes possible to see more clearly which aspects of statistical inference are universal, and which are particular to the classical or quantum domain.

Indeed, there are a number of distinct geometrical formulations of classical statistical theory, corresponding, for example, to the various $\alpha$-embeddings of Amari (see, e.g., Amari 1985 or Murray and Rice 1993), but one among these is singled out on account of its close relation to quantum theory: the geometry
of square-root density functions. This geometry is special because of the way it singles out the Levi-Civita connection on statistical submanifolds, as indicated in Proposition 2 above. In this way we are led to consider classical statistics in the language of real Hilbert space geometry, as indicated in the previous sections. The real Hilbert space formulation of standard quantum theory, on the other hand, is in itself a fairly standard construction now, though perhaps not as well known as it should be, and in the next section we shall develop some of the formalism necessary for working in this framework.

The specific point of originality in our approach is to make the link between the natural real Hilbert space arising on the one hand in connection with the classical theory of statistical inference, with the natural real Hilbert space arising on the other hand in connection with standard quantum theory. Once this identification has been made, then a number of interesting results can be seen to follow, which are explored in some detail here. In particular, the theory of classical statistical estimation can be extended directly to the quantum mechanical situation, and we are able to show how the Cramér-Rao inequality associated with a pair of canonically conjugate physical variables can be interpreted as the corresponding Heisenberg relation in the quantum mechanical context. This ties in neatly with the important line of investigation in quantum statistical estimation initiated by Helstrom (1969), Holevo (1973, 1979), and others (e.g., Yuen, Kennedy, and Lax 1975), about which we shall have more to say shortly. One of the most exciting results emerging as a by-product of our approach is the development of a series of ‘improved’ Heisenberg relations, formulated in some detail in the later sections.

8. Geometry of Quantum States

Now we turn to quantum geometry. Our goal in this section is to formulate standard quantum theory in a geometrical language that brings out more clearly its relation to the statistical geometry which we have developed in sections 2 to 6. We start with our formulation of classical inference, based on a real Hilbert space geometry, upon which we will now impose additional structure. Thus instead of ‘completely reformulating everything’ from scratch to develop a quantum statistical theory, as has conventionally been done, we shall essentially accept the classical theory, but ‘enrich’ it with some extra structure. The essential additional ingredient that we must introduce on our real Hilbert space $\mathcal{H}$, in order to study quantum mechanical systems, is, more specifically, a compatible complex structure. A complex structure on $\mathcal{H}$ is given by a tensor $J^b_a$ satisfying

$$J^b_a J^c_b = -\delta^c_a. \tag{8.1}$$

Given this structure we then say a symmetric operator $X_{ab}$ is Hermitian if it satisfies the relation

$$J^a_c J^b_d X_{ab} = X_{cd}. \tag{8.2}$$

An alternative way to express the Hermitian condition is $J^a_c X^b_b = X^a_c J^b_b$, which states that $J^a_b$ and $X^a_b$ commute. This follows from the complex structure identity (8.1) and the Hermiticity condition (8.2). We require that the complex structure be compatible with the Hilbert space structure by insisting that the metric $g_{ab}$ is Hermitian. As a consequence we have $J^a_c J^b_d g_{ab} = g_{cd}$, which is to be viewed as a fundamental relationship holding between $J^a_b$ and $g_{ab}$.
In order to proceed further it will be useful to make a comparison of the index notation being used here with the conventional Dirac notation. In the ‘real’ approach to quantum theory, state vectors are represented by elements of a real Hilbert space $\mathcal{H}$. We find that if $\xi^a$ and $\eta^a$ are two real Hilbert space vectors, then their Dirac product is given by the following complex expression:

$$
\langle \eta | \xi \rangle = \frac{1}{2} \eta^a (g_{ab} - ig_{ac}J^c_b) \xi^b .
$$

(8.3)

The Hermitian property of $g_{ab}$ implies that the tensor $\Omega_{ab} = g_{ac}J^c_b$ is automatically antisymmetric and invertible, i.e., a symplectic structure, which also satisfies the Hermitian condition in the sense that $J^a_b, J^b_a, \Omega_{ab} = \Omega_{ab}$. Since the symplectic structure $\Omega_{ab}$ is antisymmetric, it follows then that the Dirac norm agrees with the real Hilbertian norm (apart from the factor of two):

$$
\langle \xi | \xi \rangle = \frac{1}{2} g_{ab} \xi^a \xi^b .
$$

(8.4)

A real Hilbert space vector $\xi^a$ can be decomposed into complex ‘positive’ and ‘negative’ parts, relative to the specified complex structure, according to the scheme $\xi^a = \xi_+^a + \xi_-^a$, where

$$
\xi_\pm^a = \frac{1}{2} (\xi^a \mp iJ^a_b \xi^b) .
$$

(8.5)

In the case of relativistic fields, this decomposition corresponds to splitting the fields into positive and negative frequency parts, so occasionally we refer to $\xi_+^a$ and $\xi_-^a$ as the ‘positive frequency’ and ‘negative frequency’ parts of $\xi^a$. Note that $\xi_+^a$ and $\xi_-^a$ are complex ‘eigenstates’ of the $J^a_b$ operator, in the sense that $J^a_b \xi_\pm^a = \pm i \xi_\pm^a$. As a consequence, the Hermitian condition \[\xi_+^a \eta_-^b = \eta_+^a \xi_-^b\] implies that two vectors of the same ‘type’ (e.g., a pair of positive vectors) are necessarily orthogonal with respect to the metric $g_{ab}$. In other words, we have $g_{ab} \xi_\pm^a \eta_\mp^b = 0$ for any two positive (negative) vectors $\xi_\pm^a$ and $\eta_\mp^a$.

For certain purposes it is useful to introduce Greek indices to denote positive and negative parts, by writing $\xi^a = (\xi^\alpha, \xi_\alpha)$, where $\xi_\alpha$ is the complex conjugate of $\xi^\alpha$. Then, we can identify $\xi^\alpha$ with the Dirac ‘ket’ vector $|\xi\rangle$, and $\xi_\alpha$ with the complex conjugate Dirac ‘bra’ vector $\langle \xi |$, and write $\xi^a = (|\xi\rangle, \langle \xi |)$. To be more specific, a typical element in the complex Hilbert space is denoted $\psi^a$, or equivalently $|\psi\rangle$ in the conventional Dirac notation, and an element in the dual space is denoted $\varphi_\alpha = \langle \varphi |$. Hence, their inner product is written $\varphi_\alpha \psi^\alpha = \langle \varphi | \psi \rangle$. The complex conjugate of the vector $\psi^\alpha$ is $\bar{\psi}_\alpha = \langle \bar{\psi} |$, and its norm is then given by $\bar{\psi}_\alpha \psi^\alpha = \langle \bar{\psi} | \psi \rangle$. If we denote the splitting of a real Hilbert space $\mathcal{H}$ into positive and negative eigenspaces by $\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-$, then an ‘operator’ in quantum mechanics can be regarded as a linear map $T^\alpha_\beta$ from a domain in $\mathcal{H}^+$ to $\mathcal{H}^+$, given, e.g., by $T^\alpha_\beta \psi^\beta = \eta^\alpha$, for which the corresponding complex conjugate operator is $\bar{T}_\beta^\alpha = T^\alpha_\beta$. Thus, if $T$ is Hermitian, we have $T^\alpha_\beta = \bar{T}_\beta^\alpha$, and it follows that the expectation $\langle T \rangle$ of $T$ in the state $\psi$ is given by

$$
\frac{\langle \bar{\psi} | T | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\bar{\psi}_\alpha T^\alpha_\beta \psi^\beta}{\psi^\alpha \bar{\psi}_\alpha} ,
$$

(8.6)
and the variance of $T$ is
\[
\text{Var}_\psi[T] = \frac{\bar{\psi}_\alpha \tilde{T}_\alpha \bar{\psi}_\beta \psi^\beta}{\bar{\psi}_\alpha \psi_\alpha},
\] 
(8.7)
where $\tilde{T}_\alpha = T_\alpha - \langle T \rangle \delta^\alpha_\beta$. Note that $\langle \tilde{T} \rangle = 0$.

Now let us say more about the Hermitian condition. Having the decomposition $\xi_a = (\xi^\alpha, \bar{\xi}_\alpha)$ in mind, we can represent a given second rank tensor $T_{ab}$ (not necessarily symmetric, Hermitian, or real) in matrix form by writing
\[
T_{ab} = \begin{pmatrix} A_{\alpha\beta} & B_\alpha^\beta \\ C_\beta^\alpha & D_\alpha^\beta \end{pmatrix},
\] 
(8.8)
Similarly, the complex structure $J^a_b$ can be written
\[
J^a_b = \begin{pmatrix} i\delta^\alpha_\beta & 0 \\ 0 & -i\delta^\alpha_\beta \end{pmatrix},
\] 
(8.9)
Thus for the action of the complex structure tensor we find $\zeta_a \equiv J^a_b \xi_b = (i\xi^\alpha, -i\bar{\xi}_\alpha)$. In other words, the effect of $J^a_b$ is to multiply the ‘ket’ part of the given state by $i$, and the ‘bra’ part by $-i$. Moreover, it can be verified that
\[
J^c_a J^d_b T_{cd} = \begin{pmatrix} -A_{\alpha\beta} & B_\alpha^\beta \\ C_\beta^\alpha & -D_\alpha^\beta \end{pmatrix}.
\] 
(8.10)
Therefore, the requirement that the tensor $T_{ab}$ should be symmetric implies $A_{\alpha\beta} = A_{(\alpha\beta)}$, $D_{\alpha\beta} = D_{(\alpha\beta)}$, and $B_\alpha^\beta = C_\beta^\alpha$. The Hermitian condition then implies $A_{\alpha\beta} = 0$ and $D_{\alpha\beta} = 0$, and the reality condition implies $B_\alpha^\beta = \overline{C_\beta^\alpha}$. A symmetric, real Hermitian tensor $T_{ab}$ can be represented in matrix form by writing
\[
T_{ab} = \begin{pmatrix} 0 & T^\alpha_\beta \\ T^\beta_\alpha & 0 \end{pmatrix},
\] 
(8.11)
where $T^\alpha_\beta = T^\beta_\alpha$. It follows that the quadratic form $T_{ab} \xi^a \eta^b$ for a Hermitian tensor $T_{ab}$ is given by $T_{ab} \xi^a \eta^b = T^\alpha_\beta \xi^\alpha \eta^\beta + T^\beta_\alpha \xi^\beta \eta^\alpha$. In the special case of the metric $g_{ab}$ we have
\[
g_{ab} = \begin{pmatrix} 0 & \delta^\alpha_\beta \\ \delta_\alpha^\beta & 0 \end{pmatrix},
\] 
(8.12)
from which it follows that $g_{ab} \xi^a \eta^b = \xi^\alpha \eta^\alpha + \xi_\alpha \eta^\alpha$. Also, for the symplectic structure $\Omega_{ab}$ we obtain
\[
\Omega_{ab} = \begin{pmatrix} 0 & i\delta_\alpha^\beta \\ -i\delta_\alpha^\beta & 0 \end{pmatrix},
\] 
(8.13)
so that $\Omega_{ab} \xi^a \eta^b = i\xi^\alpha \eta^\alpha - i\xi_\alpha \eta^\alpha$. Clearly, we then have
\[
\xi^\alpha \eta_\alpha = \frac{1}{2} (g_{ab} + i\Omega_{ab}) \xi^a \eta^b,
\] 
(8.14)
which is consistent with equation (8.3), if we bear in mind that $\Omega_{ab}$ is antisymmetric. With these relations at hand, the reformulation in ‘real’ terms of the standard

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'complex' formalism of quantum theory can be pursued in a straightforward, systematic way. It is worth bearing in mind that in formulating quantum theory in real terms in this way we have not altered the results or physical content of the theory. These remain unchanged. Our purpose, rather, is to highlight in this way certain geometrical and probabilistic aspects of ordinary quantum mechanics that otherwise may not be obvious. For further details of the ‘real’ approach to complex Hilbert space geometry and its significance in quantum mechanics, see for example Ashtekar and Schilling (1995), Field (1996), Geroch (1971a,b), Gibbons (1992), Gibbons and Pohle (1993), Kibble (1978,1979), Schilling (1996), Segal (1947), and Wald (1976,1994).

9. Real Hilbert Space Dynamics

In this section we take the discussion further by consideration of the quantum mechanical commutation relations, as seen from a ‘real’ Hilbert space point of view. This then leads us to a natural ‘real’ formulation of the Schrödinger equation.

If $X_{ab}$ and $Y_{ab}$ are a pair of symmetric operators, then their ‘skew product’ defined by the expression $X_a Y_{ab} - X_b Y_{ba}$ is an antisymmetric tensor, and thus itself cannot represent a random variable. Nevertheless, in the case of Hermitian operators, there is a natural isomorphism between the space of symmetric tensors $X_{ab}$ satisfying $J^c_a J^d_b X_{cd} = X_{ab}$ and antisymmetric tensors $\Lambda_{ab}$ satisfying $J^c_a J^d_b \Lambda_{cd} = \Lambda_{ab}$, and the map in question is given by contraction with $J^a_b$. This follows from the fact that if $X_{ab}$ is symmetric and Hermitian, then $\Lambda_{ab} = X_{ac} J^c_b$ is automatically antisymmetric and Hermitian. Conversely, if $\Lambda_{ab}$ is antisymmetric and Hermitian, then $\Lambda_{ac} J^c_b$ is automatically symmetric and Hermitian. Thus to form the commutator of two symmetric Hermitian operators first we take their skew product, which then we multiply by the complex structure tensor to give us a symmetric Hermitian operator. After some rearrangement of terms, these results can be summarised as follows:

**Lemma 3.** The commutator $Z = i[X,Y]$ of a pair of symmetric, Hermitian operators $X$ and $Y$ is given by the symmetric Hermitian operator $Z_{ab} = (X_{ac} Y_{bd} - Y_{ac} X_{bd}) \Omega^{cd}$.

Note that the symplectic structure $\Omega_{ab}$ (or equivalently, the complex structure) is playing the role of ‘$i$’ in the relation $Z = i[X,Y]$ so as to give us a real, symmetric, Hermitian tensor $Z_{ab}$.

The anticommutator $W = \{X,Y\}$ between two symmetric operators $X_{ab}$ and $Y_{ab}$ is defined by $W_{ab} = 2X_{(a} Y_{b)c}$. This is a more ‘primitive’ operation on the space of symmetric tensors since it does not require introduction of a complex structure. The basic operator identity

$$\{\{A,B\},C\} - \{A,\{B,C\}\} = [B, [A,C]] \tag{9.1}$$

shows that even in the absence of a Hermitian structure the incompatibility between a pair of random variables can be expressed in terms of the nonassociativity of the symmetric product. In other words, we say two random variables $A$ and $C$ are compatible iff the left-hand side of (9.1) vanishes for any choice of $B$.

Now, suppose the Hamiltonian of a quantum mechanical system is represented...
by a symmetric Hermitian operator $H_{ab}$. In fact, we need $H_{ab}$ to be self-adjoint (a stronger condition), but this need not concern us for the moment. Then for the Schrödinger equation we have:

$$
\dot{\xi}^a = J^a_b H^b c c. \tag{9.2}
$$

Note that again the role of the usual ‘i’ factor is played by the complex structure tensor. Expressing this relation in terms of positive and negative parts, we then recover the conventional form of the Schrödinger equation

$$
i \dot{\xi}^a = H^a b c b, \tag{9.2}
$$

with its complex conjugate. In Dirac’s notation this is of course $i\hbar|\xi \rangle = H|\xi \rangle$.

As a consequence of (9.2) it follows at once that $\xi^a \xi_a = 0$. This is due to the Hermitian relation which says that $J_{ac} H^c b$ is antisymmetric. Thus, as expected, the Schrödinger equation respects the normalisation $g_{ab} \xi^a \xi^b = 1$.

Having formulated the conventional quantum dynamics in terms of real Hilbert space, we are in a position to make an interesting link with statistical considerations. To begin, we note that the usual phase freedom in quantum mechanics can be incorporated by modifying the Hamiltonian according to the prescription

$$H^b b \rightarrow \tilde{H}^b b = H^b b + \varphi^b a. \tag{9.3}
$$

We can take advantage of this freedom by consideration of the following result.

**Proposition 10.** There is a unique choice of phase such that the tangent vector $\dot{\xi}^a$ of the dynamical trajectory is everywhere orthogonal to the direction $\xi = J^a \xi^b$. This choice of $\varphi$ minimises the Fisher information $4g_{ab} \xi^a \xi^b$.

In fact, the relevant phase factor is given by $\varphi = -H_{ab} \xi^a \xi^b / \xi^c \xi_c$. Physically, this choice of phase fixing implies an adjustment of the mean of the Hamiltonian.

Clearly, we have $\tilde{H}_{ab} \xi^a \xi^b = 0$, and it is not difficult to see that the same choice of $\varphi$ minimises $4g_{ab} \dot{\xi}^a \dot{\xi}^b$. In fact, for general $\varphi$ we have $g_{ab} \dot{\xi}^a \dot{\xi}^b = g_{ab} H^a b \xi^c \xi^d + 2\varphi H_{ab} \xi^a \xi^b + \varphi^2 g_{ab} \xi^a \xi^b$, from which it follows at once that $g_{ab} \dot{\xi}^a \dot{\xi}^b$ is minimised for the choice of $\varphi$ indicated. This result will be used extensively in our work on quantum estimation. With this choice of phase the modified Schrödinger equation reads

$$
\dot{\xi}^a = J^a_b \tilde{H}^b c c, \tag{9.3}
$$

where

$$
\tilde{H}_{ab} = H_{ab} - \left( \frac{H_{cd} \xi^c \xi^d}{\xi^e \xi_e} \right) g_{ab} \tag{9.4}
$$

represents now the deviation of the Hamiltonian from its mean, in accordance with the notation introduced earlier. Note that for the state defined by $\xi = J^a_b \xi^b$, the dynamical equation becomes $\dot{\xi}^a = J^a_b \tilde{H}^b c c$, since $J^b_a$ commutes with $H^a b$. Thus, $\xi^a$ also satisfies the Schrödinger equation. We can think of the complex projective space (in general infinite dimensional) formed by projectivising the ‘positive’ Hilbert space $H^+$ as being the ‘true’ space of pure states. Then the essence of Proposition [10] is that there is a unique ‘lift’ from this projective space $P(H^+)$ to the real Hilbert space $H$ such that the tangent vector $\dot{\xi}^a$ is everywhere orthogonal to both $\xi^a$ and $\tilde{\xi}^a$.

As a matter of interpretation we make the following observation regarding the ‘modified’ Schrödinger equation. In the standard treatment of quantum mechanics one is taught that the time independent Schrödinger equation is given

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by $H|\xi\rangle = E|\xi\rangle$, whereas the time dependent case can be written by use of
the correspondence principle $E \leftrightarrow i\partial_t$. Although generally accepted, the basis
of this correspondence has to be regarded as somewhat mysterious, and to that
extent also unsatisfactory. Now, in the modified Schrödinger equation we have
$i\partial_t|\xi\rangle = (H - \langle H \rangle)|\xi\rangle$. Hence if the state is time independent, we recover the
usual time independent equation $(H - E)|\xi\rangle = 0$. In this way, we do not have
to specify which representation of the canonical commutation relations we work
with. While in general terms the theory is independent of the specific choice of
phase, it seems that there is a unique choice of phase that makes everything fit
in well from a physical point of view, and interestingly we are led to the same
result from purely statistical considerations.

Now suppose $B_{ab}$ is a symmetric Hermitian operator and we write $B(t) :=
E_{\xi(t)}[B]$ for the expectation

$$E_{\xi(t)}[B] = \frac{B_{ab}\xi^a(t)\xi^b(t)}{g_{cd}\xi^c(t)\xi^d(t)},$$

where $\xi^a(t)$ satisfies the modified Schrödinger equation (9.3), or equivalently,
$\xi^a(t) = \exp[tJ^a_bH^b_c]\xi^c(0)$, where $\xi^c(0)$ is the state vector at $t = 0$. Thus $B(t)$
represents the expectation of $B_{ab}$ along the given trajectory. It follows that

$$\frac{dB(t)}{dt} = \frac{C_{ab}\xi^a\xi^b}{g_{cd}\xi^c\xi^d},$$

along $\xi^a(t)$, where $C_{ab} = (B_{ac}H_{bd} - H_{ac}B_{bd})\Omega^{cd}$ is the commutator between $B_{ab}$
and $H_{ab}$. This is the ‘real’ version of the familiar relation $d\langle B \rangle/dt = i\langle [B, H] \rangle$.
It is important to note that use of the ‘modified’ Schrödinger equation does not
affect this result.

If $P_{ab}$ and $Q_{ab}$ are symmetric Hermitian operators satisfying the commutation
relation

$$(P_{ac}Q_{bd} - Q_{ac}P_{bd})\Omega^{cd} = g_{ab},$$

then we say that $P_{ab}$ is canonically conjugate to $Q_{ab}$, and we refer to (9.7) as
the Heisenberg canonical commutation relation. This would apply, for example,
when $P_{ab}$ and $Q_{ab}$ are the self-adjoint position and momentum operators of a
quantum system. In fact, the Heisenberg commutation relation (9.7) has to be
regarded to some degree as formal, since the domain in $\mathcal{H}$ over which (9.7)
is valid is not necessarily obvious. This point can be remedied by consideration of
the Weyl relation, which offers a more general and, ultimately, more rigorous
basis for formulating the concept of canonical conjugacy. In real terms the Weyl
relation is given by

$$\exp[-qJ^a_bP^b_c]\exp[pJ^a_dQ^d_e] = \exp[pJ^a_b(Q^b_c + q\delta^b_c)]\exp[-qJ^c_dP^d_e],$$

where $p$ and $q$ are parameters. Note that in the Weyl relation the effect of inter-
changing the two terms on the left is to ‘shift’ the operator $Q^a_b$ by the amount
$q\delta^a_b$. The Heisenberg commutation relation (9.7) is then obtained by formally
differentiating (9.8) with respect to $p$ and $q$, then setting them to zero.

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10. Quantum Measurement

We shall now turn to the problem of parametric estimation for quantum mechanical states. By expressing quantum theory within a real Hilbert space framework, and studying the corresponding ‘real dynamics’, we take advantage of the geometrical formulation of statistical inference outlined earlier. We begin with some remarks indicating the general setting for our investigations in quantum measurement and quantum statistical estimation. In particular, with a view to the parameter estimation problem we shall be considering shortly, it will suffice for our purposes to examine the case where we are concerned with the measurement of an observable with a continuous spectrum, such as position or momentum.

We shall consider the situation where the system is in a pure state, characterised in real terms by a state vector $\xi^a$ in a real Hilbert space $\mathcal{H}$ equipped with an inner product $g_{ab}$ and a compatible complex structure $J^a_b$. It is possible also to consider the case where the state is described by a general density matrix, but this is not required for present purposes.

The measurement of an observable is fully characterised in quantum mechanics by the specification of a resolution of the identity. By this we mean a one-parameter family $M_{ab}(x)$ of positive symmetric Hermitian operators that integrate up to form the identity operator. Thus we have $M_{ab} = M_{ba}$, $M_{ab}\xi^a\xi^b \geq 0$ for any vector $\xi^a \in \mathcal{H}$, $M_{cd}J^c_aJ^d_b = M_{ab}$, and

$$\int_{-\infty}^{\infty} M_{ab}(x)dx = g_{ab}. \quad (10.1)$$

Then the probability that the observable $X$ represented by the measurement $M_{ab}(x)$ lies in the interval $\alpha < x < \beta$, if the state of the system is $\xi^a$, is given by

$$\text{Prob}[\alpha < x < \beta] = \int_{\alpha}^{\beta} M_{ab}(x)\xi^a\xi^b dx, \quad (10.2)$$

and for the expectation of $X$ we have

$$E_{\xi}[X] = \int_{-\infty}^{\infty} xM_{ab}(x)\xi^a\xi^b dx. \quad (10.3)$$

The observable $X_{ab}$ itself, on the other hand, is given by

$$X_{ab} = \int_{-\infty}^{\infty} xM_{ab}(x)dx, \quad (10.4)$$

from which it follows that $E_{\xi}[X] = X_{ab}\xi^a\xi^b$. The probability law $p(x|\xi)$ is not readily ascertainable from the operator $X_{ab}$ directly, and this is why one needs the resolution of the identity $M_{ab}(x)$, or equivalently, the density function

$$p(x|\xi) = M_{ab}(x)\xi^a\xi^b \quad (10.5)$$

for the random variable $X$, conditional on the specification of the state $\xi^a$.

It is interesting to note the relationship between properties of the operator $X_{ab}$ defined by the spectral resolution $M_{ab}(x)$ and the corresponding resolution of the identity $M_{ab}(x)$. If $X_{ab}$ is a bounded operator, which is to say that there exists a constant $c$ such that $|X_{ab}\xi^a\xi^b| \leq cg_{ab}\xi^a\xi^b$ for all $\xi^a \in \mathcal{H}$, then there exists a unique spectral resolution $M_{ab}(x)$ with the following two additional properties: i) the resolution is orthogonal, or projection valued, in the sense that
More generally, if \( X_{ab} \) is self-adjoint (but not necessarily bounded) then there exists a unique orthogonal resolution of unity \( M_{ab}(x) \) such that \( X_{ab} \) is given by \((10.4)\), and that the domain of the operator \( X_{ab} \) consists of all vectors \( \xi^a \) satisfying

\[
\int_{-\infty}^{\infty} x^2 M_{ab}(x) \xi^a \xi^b dx < \infty. \tag{10.6}
\]

On the other hand, if \( X_{ab} \) is maximally symmetric, then there exists a unique resolution \( M_{ab}(x) \) such that \( X_{ab} \) has the spectral representation \((10.4)\), and the expectation of its square is given by

\[
X^c_a X^c_b \xi^a \xi^b = \int_{-\infty}^{\infty} x^2 M_{ab}(x) \xi^a \xi^b dx \tag{10.7}
\]

for any state \( \xi^a \) in the domain of \( X_{ab} \), which is given by \((10.6)\). In this case the resolution of the identity is not orthogonal.

In noting these results we recall that the domain \( D(X) \) of a densely defined operator \( X_{ab} \) consists of those state vectors \( \xi^a \) for which \( X_{ab} \xi^b \) exists, or equivalently, for which \( X^c_a X^c_b \xi^a \xi^b < \infty \). If \( X_{ab} \xi^a \eta^b = X_{ab} \eta^a \xi^b \) for all \( \xi^a, \eta^a \in D(X) \), then we say \( X_{ab} \) is symmetric, and write \( X_{ab} = X_{ba} \). Then we define the adjoint domain \( D^*(X) \) to consist of all those vectors \( \eta^a \) for which there exists a vector \( \zeta^a \) such that \( \eta^a(X_{ab} \xi^b) = \zeta^a \xi^b \) for every \( \xi^a \) in \( D(X) \). For any element \( \eta^a \in D^*(X) \) we thus define the adjoint operator \( X_{ab}^* \), with domain \( D^*(X) \), by the action \( X_{ab}^* \eta^b = \zeta^a \). If \( D(X) = \mathcal{H} \), then \( X_{ab} \) bounded; if \( D(X) = D^*(X) \) then we say \( X_{ab} \) is self-adjoint.

For a symmetric operator, \( D(X) \subseteq D^*(X) \). If \( D(X) \subseteq D(Y) \) and if \( X_{ab} = Y_{ab} \) on \( D(X) \), then we say \( Y_{ab} \) is an extension of \( X_{ab} \). An operator is said to be maximally symmetric if it is symmetric, but has no self-adjoint extension. See, e.g., Bogolubov, et. al. (1975) or Reed and Simon (1974) for further details.

Perhaps it can be stated that one of the most important modern developments in the understanding of basic quantum theory was the realisation that general measurements are given by positive operator-valued measures (POM), which involve general, nonorthogonal resolutions of the identity in an essential way. At the same time, one has to understand the category of observables in quantum mechanics to be widened on that basis to include maximally symmetric operators, as opposed to merely self-adjoint operators. See, e.g., Davies and Lewis (1970), Helstrom (1969), and Holevo (1973, 1979).

We note this because some of the most interesting parameter estimation problems in quantum statistical inference involve nonorthogonal resolutions—for example, time and phase measurement—for which the relevant estimators are maximally symmetric operators characterised by nonorthogonal resolutions.

In what follows we shall be particularly concerned with measurements associated with one-parameter families of unitary transformations. In this connection we point out that a transformation \( \xi^a \rightarrow O^a_b \xi^b \) represents a general rotation of the real Hilbert space \( \mathcal{H} \) about its origin if \( O^a_c O^b_d g_{ab} = g_{cd} \). A unitary transformation \( \xi^a \rightarrow U^a_b \xi^b \) is characterised by an operator \( U^a_b \) that is both orthogonal, in the sense that the metric is preserved, and symplectic, in the sense that the symplectic structure \( \Omega_{ab} \) is also preserved, so \( U^a_c U^b_d \Omega_{ab} = \Omega_{cd} \). This gives us a characterisation of unitary transformations in purely real terms.

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Now suppose $U^a_b(\theta)$ is a continuous one-parameter family of unitary transformations on $\mathcal{H}$, satisfying $U^a_b(\theta)U^c_d(\theta') = U^a_b(\theta + \theta')$. Then there exists a self-adjoint operator $F_{ab}$ such that $U^a_b(\theta) = \exp[\theta J^a_{b}F_{b}^c]$. For example, if $P_{ab}$ is the momentum operator in a specific direction, then $U^a_b(\theta) = \exp[\theta J^a_{b}P_{b}^c]_F$ can be interpreted as a `shift' operator, and the one-parameter family of states $\xi^a(\theta) = U^a_b(\theta)\xi^b$ is obtained by shifting the states along the given axis. The question arises then, given such a family $\xi^a(\theta)$, what measurements can we perform to determine the relation of the true state of the system to the original state $\xi^a$?

A resolution of the identity $M_{ab}(x)$ is said to be covariant with respect to the one-parameter family of unitary transformations $U^a_b(\theta)$ if

$$U^c_d(\theta)U^d_b(\theta)M_{cd}(x) = M_{ab}(x - \theta).$$

(10.8)

In that case it is straightforward to verify that the symmetric operator $\Theta_{ab}$ defined by

$$\Theta_{ab} = \int_{-\infty}^{\infty} (x - \mu)M_{ab}(x)dx,$$

(10.9)

where $\mu = \Theta_{ab}\xi^a\xi^b/\xi^a\xi^c$, is an unbiased estimator for the parameter $\theta$ in the sense that

$$\frac{\Theta_{ab}\xi^a(\theta)\xi^b(\theta)}{g_{cd}\xi^c(\theta)\xi^d(\theta)} = \theta$$

(10.10)

for any state vector $\xi^a(\theta)$ along the specified trajectory.

In particular, one can verify that if the symmetric operator $\Theta_{ab}$ is canonically conjugate to $F_{ab}$, then its spectral resolution $M_{ab}(x)$ necessarily satisfies the covariance relation (10.8). A symmetric operator $\Theta_{ab}$ is defined to be canonically conjugate to a self-adjoint operator $F_{ab}$ if for all values of the parameters $\theta, \phi$ we have

$$\exp[-\theta J^a_{b}F_{c}]\exp[\phi J^a_{d}F_{e}]\exp[\theta J^e_{f}F_{g}] = \exp[\phi J^a_{d}(\Theta_{g} + \theta\delta_{g})].$$

(10.11)

In other words, the unitary transformation $U^a_b(\theta)$ has the effect of shifting $\Theta_{b}^a$ by the amount $\theta\delta_{b}^a$ in (10.11). If $F_{ab}$ and $\Theta_{ab}$ are self-adjoint, then the exponentials in (10.11) can be given meaning by a spectral representation, and (10.11) is equivalent to the Weyl relation. On the other hand, it may be that the given self-adjoint operator $F_{ab}$ has no self-adjoint canonical conjugate. Nevertheless there may exist a maximally symmetric operator $\Theta_{ab}$ satisfying (10.11), if we define

$$\exp[\phi J^a_{d}\Theta_{c}] := \int_{-\infty}^{\infty} \left[ \cos(\phi x)\delta_{b}^a + \sin(\phi x)J^a_{b} \right] M_{ab}(x)dx,$$

(10.12)

where $M_{ab}(x)$ is the unique spectral resolution for $\Theta_{ab}$ satisfying the required conditions on its first and second moments. This occurs, for example, in the case of a Hermitian operator that is bounded below, which admits no self-adjoint canonical conjugate, but nevertheless under fairly general conditions admits a maximally symmetric canonical conjugate satisfying (10.11).

Consider, for example, the case of a free particle in one dimension, for which the momentum and position operators are denoted $P$ and $Q$, and the Hamiltonian is $H = P^2/2m$. Then, $H$ has no self-adjoint canonical conjugate, but it does have a well defined maximally symmetric canonical conjugate, given (Holevo 1982) by

$$T = i\text{m} \text{sign}(P)|P|^{-1/2}Q|P|^{-1/2},$$

(10.13)
and it is not difficult to check, at least formally, that \( TH - HT = i \).

If we work in the usual momentum representation, for which the wave function is given by \( \xi(p) \), assumed normalised, then \( D(T) \) is given by those functions for which

\[
\int_{-\infty}^{\infty} \left| \frac{d\xi(p)}{dp} \right| |p|^{-1/2} |p|^{-1} dp < \infty.
\]

(10.14)

If \( \xi(p,t) \) is a one-parameter family of states satisfying the Schrödinger equation \( i\partial_t \xi = H\xi \), we find that

\[
\langle \xi(t)|T|\xi(t)\rangle = t + \langle \xi(0)|T|\xi(0)\rangle,
\]

which shows that \( T \) is an estimator for \( t \). We mention this example to illustrate the point that even in a simple situation, the construction of the relevant estimator can be a subtle matter.

11. Quantum Estimation

Suppose now we consider a family of normalised state vectors \( \xi^a(t) \), parameterised by the time \( t \), that satisfy the Schrödinger equation (9.3). The curve \( \xi^a(t) \) lies on the unit sphere \( S \) in the real Hilbert space \( \mathcal{H} \), and is characterised by the fact that it is the unique lift of the quantum mechanical state trajectory in the complex projective Hilbert space to the sphere \( S \) with the property that it is everywhere orthogonal to the direction \( \xi^a = J^a_b \xi^b \), as indicated in Proposition 10 (cf. figure 1). Regarding this curve as a statistical manifold, we shall study the problem of estimating the time parameter \( t \) by use of the geometric techniques developed in §§2-5. Let \( T_{ab} \) denote an unbiased estimator for \( t \). Thus \( T_{ab} \) is a real symmetric Hermitian operator satisfying

\[
T_{ab} \xi^a(t) \xi^b(t) = t,
\]

(11.1)

for a system that is in the state \( \xi(t) \). For example, if \( T_{ab} \) is maximally symmetric and canonically conjugate to \( H_{ab} \), then by the argument of the previous section we can make an adjustment of the form \( T_{ab} \rightarrow T_{ab} + kg_{ab} \) for a suitable constant \( k \) to remove the bias of \( T_{ab} \), which does not change the conjugacy condition, and we are left with an estimator satisfying (11.1).

Our idea is to apply the generalised Bhattacharyya bounds established in §5 to the quantum mechanical estimation problem, and consider the possibility of establishing sharper variants of the Heisenberg uncertainty relations \( \Delta H \Delta T \geq 1/2 \) in the case of canonically conjugate variables.

The geometrical content of the generalised Bhattacharyya bound is that given the normal vector \( \nabla_a t \) to the time-slice surfaces, we can choose a set of orthogonal vectors in \( \mathcal{H} \) and express the length of this vector in terms of its orthogonal components. Then by use of Proposition 6 we can formulate a set of bounds on the variance of \( T_{ab} \). In the ‘classical’ setting for parameter estimation in §5, we found it natural to consider the orthogonal vectors given by \( \xi^{(k)}_a \) \( (k = 1, 2, \ldots) \), the \( k \)-th derivatives of the states \( \xi_a \) projected orthogonally to the lower order derivatives. These satisfy \( g^{ab} \xi^{(k)}_a \xi^{(k)}_b = 0 \) for \( j \neq k \), and will be referred to as the ‘classical system’ of orthogonal vectors. In the quantum mechanical situation, the resulting scheme of possible sets of orthogonal vectors is somewhat richer, since the complex structure tensor can also be brought into play. In particular,
we find that the Cauchy-Riemann field $\zeta^a = J^a_b \xi^b$ is orthogonal to $\xi^a$, $\zeta^a$ is orthogonal to $\dot{\xi}^a$, and so on. Therefore, we can construct a set of orthogonal vectors given in terms of $\xi^a, \zeta^a$, and their higher order derivatives. These will be referred to as the ‘quantum system’ of orthogonal vectors, and denoted $\tilde{\zeta}^{(k)}_a$ and $\zeta^{(k)}_a$ ($k = 0, 1, 2, \cdots$), characterised by the property that $\tilde{\zeta}^{(j)}_a \zeta^{(k)}_a g^{ab} = 0$, $\xi^{(j)}_a \zeta^{(k)}_a g^{ab} = 0$, and $\zeta^{(j)}_a \tilde{\zeta}^{(k)}_a g^{ab} = 0$, for $j \neq k$.

Before considering the higher order terms, we study the two lowest order terms arising from the quantum system, to note the familiar inequalities from standard quantum mechanics thus arising. In this case, the variance bound is:

$$\text{Var}_\xi[T] \geq \frac{(\dot{\xi}^a \nabla_a t)^2}{4 \xi^b \xi_b} + \frac{2 \xi^a \nabla_a t}{4 \xi^b \xi_b} .$$

(11.2)

**Proposition 11.** Let $\xi^a(t)$ satisfy the modified Schrödinger equation (11.3), and set $\zeta^a = J^a_b \xi^b$. Let $T_{ab}$ be an unbiased estimator for $t$. Then, $\dot{\xi}^a \nabla_a t = 1$, and $\dot{\xi}^a \nabla_a t = -2 \text{Cov}_\xi[H, T]$, where $\text{Cov}_\xi[H, T]$ denotes the covariance of the operators $H_{ab}$ and $T_{ab}$ in the state $\xi^a$.

The proof is as follows. The fact that $\dot{\xi}^a \nabla_a t = 1$ follows directly from the chain rule. Alternatively, notice that differentiation of (11.1) with respect to $t$ implies, by use of (11.3), that

$$\frac{2 T_{ac} H_{bd} \Omega^{cd} \xi^a \xi^b}{g_{ab} \xi^a \xi^b} = 1 \quad (11.3)$$

for any state vector on the specified trajectory $\xi^a(t)$. On the other hand, $\dot{\xi}^a \nabla_a t = J^a_b \dot{H}^b_c \xi^c \nabla_a t$ by (9.3), and

$$\nabla_a t = \frac{2 T_{ab} \xi^b}{g_{cd} \xi^c \xi^d} , \quad (11.4)$$

which taken together with (11.3) imply $\dot{\xi}^a \nabla_a t = 1$, as required. It follows then from the definition of $\zeta^a$ together with (9.3) and (8.1) that $\zeta = -\dot{H}_{ab} \xi^a \xi^b$. Thus we have $\dot{\xi}^a \nabla_a t = -2 \dot{H}_{ac} \xi^a \xi^b / \xi^c \xi^c$, which by virtue of the definition of covariance given in §2 leads to the result $\dot{\xi}^a \nabla_a t = -2 \text{Cov}_\xi[H, T]$.

Therefore, if we write $\Delta_\xi T^2 := \langle |(T^2 - \langle T^2 \rangle_\xi) \rangle \rangle$ for the variance of the estimator $T$, then, for the lowest order terms in the quantum variance bound, the inequality (11.2) reads

$$\Delta_\xi T^2 \Delta_\xi H^2 \geq \frac{1}{4} + \text{Cov}_\xi[H, T] .$$

(11.5)

In obtaining this result we have used the fact that the Fisher information in (11.2) is given by: $G = 4 \xi^a \dot{\xi}_a = 4 J^a_c \xi^b \dot{H}_{c d} \xi^e \dot{H}_{f j} \xi_j \xi^f = 4 H_c \dot{H}_a \xi^a \xi^b - 4 (H_{ab} \xi^a \xi^b)^2 = 4 \Delta_\xi H^2$, where $\Delta_\xi H^2 = \text{Var}_\xi[H]$ is the variance of the Hamiltonian (squared energy uncertainty) in the state $\xi^a$. In this way, we recover the standard ‘textbook’ account of the uncertainty relations (see, e.g., Isham 1995). In particular, the second term on the right of (11.5) is usually represented by an anticommutator.
via the relation
\[\text{Cov}_\xi[H, T] = \frac{1}{2}E_\xi[\hat{H}\hat{T} + \hat{T}\hat{H}], \quad (11.6)\]
where \(\hat{H} = H - E_\xi[H]\) and \(\hat{T} = T - E_\xi[T]\). If we omit the second term in (11.5) and keep the first term, corresponding to a quantum extension of the standard Cramér-Rao lower bound (11.2), we find
\[\Delta_\xi T^2 \Delta_\xi H^2 \geq \frac{1}{4}. \quad (11.7)\]

The statistical interpretation of this result is as follows. Suppose we are told that at \(t = 0\) a quantum mechanical system is in the state \(\xi^a(0)\), and it evolves subsequently according to the Schrödinger equation, with a prescribed Hamiltonian. Some time later we are presented with the system (or perhaps a large number of independent, identical copies of it), and we are required to make a measurement (or a set of identically designed measurements on all the copies) to determine \(t\). The measurement is given by an observable \(T_{ab}\) characterised by a nonorthogonal resolution of the identity \(M_{ab}(x)\). The probability that the result \(T\) of a given measurement lies in the range \((\alpha, \beta)\) is
\[\text{Prob}[\alpha < T < \beta] = \int_\alpha^\beta M_{ab}(x)\xi^a(t)\xi^b(t)dx,\]
and for the expectation of \(T\) we have \(E_{\xi(t)}[T] = t\). Thus, by averaging the results on all the copies we can approximate the value of \(t\). The variance of \(T\) is necessarily bounded from below, in accordance with (11.7). On the other hand, the variance of the average of the results on \(n\) copies is \(n^{-1}\Delta_\xi T^2\). Hence, by making repeated measurements on different copies of the system we can improve the reliability of the estimate for \(t\), despite the uncertainty principle.

12. Higher Order Quantum Variance Bounds

Some general remarks are in order concerning the relations (11.5). We note that although the first term in (11.5) is independent of the specific choice of estimator, the second term involving the covariance between \(H_{ab}\) and \(T_{ab}\) depends on the choice of \(T_{ab}\). Hence this term is often dropped in the consideration of uncertainty relations, although in general the bound must be sharper than what we have in (11.7). On the other hand, the reader may have observed that in deriving (11.3) we have not, in fact, assumed that \(T_{ab}\) is canonically conjugate to \(H_{ab}\). We have merely assumed that \(T_{ab}\) is an estimator for \(t\), for the given trajectory \(\xi^a(t)\), in accordance with (11.4). This is a weaker condition than canonical conjugacy, and thus it is legitimate to enquire whether, under the assumption of canonical conjugacy, it might be possible to derive bounds sharper than (11.7), but nevertheless independent of the specific choice of estimator. Therefore, following the general approach outlined in §5, we propose to study contributions from higher order Bhattacharyya type corrections to the CR lower bound to search for such terms. We find is that some of the corrections depend upon the choice of \(T_{ab}\), while others do not. Those terms that are independent of the choice of the estimator contribute to a set of generalised Heisenberg relations for quantum statistical estimation.

Before investigating details, we present some general results useful in obtaining higher order corrections. We assume that the state trajectory \(\xi^a\) satisfies the dynamical equation (9.3).
Lemma 4. Let $\xi^{(n)a}$ denote the $n$-th derivative of $\xi^a$ with respect to the time parameter $t$. Then, $g_{ab}\xi^{(n)a}\xi^{(n)b} = \langle \hat{H}^{2n} \rangle$, where $\langle \hat{H}^r \rangle$ denotes the $r$-th moment of the Hamiltonian about its mean.

This follows directly by differentiation of the Schrödinger equation (12.3), and use of the Hermiticity condition for the metric $g_{ab}$. An example for $n = 1$ is given by the expression $G = 4g_{ab}\xi^{a}\xi^{b} = 4\langle \hat{H}^2 \rangle$ for the Fisher information.

Lemma 5. For a Schrödinger state $\xi^a$, the even moments of the Hamiltonian about its mean are independent of the time parameter.

Indeed, since $\langle \hat{H}^{2n} \rangle = g_{ab}\xi^{(n)a}\xi^{(n)b}$, we obtain $\partial_t\langle \hat{H}^{2n} \rangle = 2\xi^{(n)a}g_{ab}J^a_{c}\hat{H}_{d}^{c}\xi^{(n)d}$, which vanishes. An elementary consequence of this result is that for arbitrary $n$ we have:

$$g_{ab}\xi^{(n+1)a}\xi^{(n)b} = 0. \quad (12.1)$$

A remarkable result which is essential in finding higher order corrections that are independent of the choice of $T$ is the following.

Proposition 12. Let $T_{ab}$ be canonically conjugate to $H_{ab}$, and hence an unbiased estimator for the parameter $t$. Then

$$T_{ab}\xi^{(n)a}\xi^{(n)b} = t g_{ab}\xi^{(n)a}\xi^{(n)b} + k, \quad (12.2)$$

where $k$ is a constant. Thus for each $n$, $\hat{T}_{ab}\xi^{(n)a}\xi^{(n)b}$ is a constant of the motion along the Schrödinger trajectory.

Proof. We recall from (12.1) that $T_{ab}$ is canonically conjugate to $H_{ab}$ if $(T_{ac}H_{bd} - H_{ac}T_{bd})\Omega^{cd} = g_{ab}$, a relation which can also be written in the symmetric form

$$(T_{ac}H_{bd} + T_{bc}H_{ad})\Omega^{cd} = g_{ab}. \quad (12.3)$$

Now suppose we differentiate $T_{ab}\xi^{(n)a}\xi^{(n)b}$. The Schrödinger equation in the form $\dot{\xi}^a = \Omega^{ac}\hat{H}_{cd}\xi^d$ implies $\dot{\xi}^{(n)a} = \Omega^{ac}\hat{H}_{cd}\xi^{(n)d}$, and thus

$$\partial_t(T_{ab}\xi^{(n)a}\xi^{(n)b}) = 2T_{ab}\Omega^{ac}\hat{H}_{cd}\xi^{(n)d}\xi^{(n)b}. \quad (12.4)$$

Since $T_{ab}\Omega^{ac}\hat{H}_{cd}\xi^{(n)d}\xi^{(n)b}$ vanishes automatically, we can replace the $\hat{H}_{cd}$ on the right-hand side of (12.4) with $H_{cd}$. However, according to (12.3) we have

$$2T_{ab}\Omega^{ac}\hat{H}_{cd}\xi^{(n)d}\xi^{(n)b} = g_{bd}\xi^{(n)b}\xi^{(n)d}. \quad (12.5)$$

On the other hand, Lemma 3 says that $g_{ab}\xi^{(n)a}\xi^{(n)b}$ is independent of $t$. Thus by integration of (12.4) we obtain the desired result.

Lemma 6. Let $T_{ab}$ be canonically conjugate to $H_{ab}$. Then for odd integers $n$, with $m = (n - 1)/2$, we have:

$$2T_{ab}\xi^{a(n)}\xi^{b} = (-1)^m n g_{ab}\xi^{(m)a}\xi^{(m)b}. \quad (12.6)$$

We sketch the derivation of this result. First, for $n = 1$, it follows from $T_{ab}\xi^{a}\xi^{b} = t$ that $2T_{ab}\dot{\xi}^{a}\xi^{b} = 1$.

By differentiating this twice, we find $T_{ab}\ddot{\xi}^{a}\xi^{b} + 3T_{ab}\dot{\xi}^{a}\dot{\xi}^{b} = 0$. On the other
hand, it follows from Proposition [12] that \( T_{ab} \dot{\xi}^a \dot{\xi}^b = t \dot{\xi}^a \dot{\xi} + k \). Formula (12.1) then allows us to deduce that \( 2T_{ab} \ddot{\xi}^a \ddot{\xi}^b = \dot{\xi}^a \dot{\xi}^b \). This gives us the desired result in the case \( n = 3 \), namely: \( 2T_{ab} \ddot{\xi}^a \ddot{\xi}^b = -3 \dot{\xi}^a \dot{\xi} \).

If we differentiate \( T_{ab} \ddot{\xi}^a \ddot{\xi}^b = t \) five times, we obtain \( T_{ab} \dddot{\xi}^{(5)a} \dddot{\xi}^b = -5T_{ab} \dddot{\xi}^{(4)a} \dddot{\xi}^b - 10T_{ab} \dddot{\xi}^{(3)a} \dddot{\xi}^b \). Then differentiating \( 2T_{ab} \dddot{\xi}^a \dddot{\xi}^b = \dddot{\xi}^a \dddot{\xi} b \) twice, we find \( T_{ab} \dddot{\xi}^{(4)a} \dddot{\xi}^b = -3T_{ab} \dddot{\xi}^{(3)a} \dddot{\xi}^b \), from which it follows that \( T_{ab} \dddot{\xi}^{(5)a} \dddot{\xi}^b = 5T_{ab} \dddot{\xi}^a \dddot{\xi}^b \). However, since \( T_{ab} \dddot{\xi}^a \dddot{\xi} b = t \dddot{\xi}^a \dddot{\xi} + k \), we deduce by use of (12.1) that \( 2T_{ab} \dddot{\xi}^a \dddot{\xi} b = \dddot{\xi}^a \dddot{\xi} \), and the desired result follows for \( n = 5 \), namely: \( 2T_{ab} \dddot{\xi}^{(5)a} \dddot{\xi} b = 5 \dddot{\xi}^a \dddot{\xi} \). Higher order formulae can be deduced analogously.

Armed with these results we are now in a position to deduce some higher order corrections to the Heisenberg relations for canonically conjugate observables. Again, we consider the measurement problem for the parameter \( t \) in the case of a one-parameter family of state vectors \( \xi^n(t) \) generated by the Schrödinger evolution (9.3), with a given Hamiltonian \( H_{ab} \). The observable \( \frac{\partial}{\partial t} \) is defined by

\[
\tilde{\xi}^a(t) = \frac{\partial}{\partial t} \xi^a(t).
\]

Formula (12.1) and the Hermitian condition (5.2) for \( H_{ab} \) that the norms of \( \tilde{\xi}^2a \) and \( \tilde{\xi}^2a \) agree, and are given by

\[
\xi^2a = \xi^a - \frac{\dot{\xi}^a \dot{\xi}^b}{\xi^c} \xi^c - \frac{\ddot{\xi}^a \ddot{\xi}^b}{\xi^c} \xi^c.
\]

Here we have used the fact that in order to obtain the second order (quantum) system of orthogonal vectors, we subtract the components of lower order derivatives of \( \xi^a \) and \( \xi^a \) from \( \dddot{\xi}^a \) and \( \dddot{\xi}^a \). There are only three terms appearing in these expressions since \( \dddot{\xi}^a \dot{\xi}^a = \dddot{\xi}^a \dot{\xi}^a = \dddot{\xi}^a \dot{\xi}^a = 0 \) and \( \dddot{\xi}^a \dddot{\xi}^a = \dddot{\xi}^a \dddot{\xi}^a = 0 \). It can be verified by use of (12.1) and the Hermitian condition (5.2) for \( H_{ab} \) that the norms of \( \tilde{\xi}^2a \) and \( \tilde{\xi}^2a \) agree, and are given by

\[
\xi^2a = \xi^a - \frac{\dot{\xi}^a \dot{\xi}^b}{\xi^c} \xi^c - \frac{\ddot{\xi}^a \ddot{\xi}^b}{\xi^c} \xi^c.
\]

We note that \( K_\xi^2 \) is the curvature of the corresponding classical ‘thermal’ state defined by the differential equation

\[
\frac{\partial \psi^a}{\partial \beta} = -\frac{1}{2} H_{ab} \psi^b.
\]
The term ‘thermal state’ used in this context is meant to suggest that we identify the parameter in the differential equation (12.12) with the inverse temperature $\beta$ (Brody and Hughston 1996d, 1997a). It is interesting to note that the Schrödinger trajectories form a family of curves orthogonal to the corresponding classical thermal state trajectories, i.e., wherever they meet we have $\psi^a_\xi a = 0$. According to the argument outlined in §4, a thermal trajectory comprises an exponential family of distributions. However, since $\Omega_{ab} H^c_{\beta}$ is antisymmetric, the Schrödinger equation does not generate an exponential family in the $t$ variable.

The first two terms on the right of (12.7) lead, as we have seen, to the standard first order uncertainty relation (11.3). Now we proceed to value the second order terms. The numerators appearing in the second term of (12.13) can be calculated as follows. We consider the term involving $\xi^{(2)a}$ first. By use of (11.4) and (12.8), and the fact that $\xi^{(2)a} \xi^b_{gab} = 0$, this can be seen to be given by four times the square of the expression

$$
\left( \xi^a - \frac{\langle \tilde{c} b \tilde{c}_b \rangle}{\xi^c \xi^c} \xi^a - (\tilde{c} b \xi^b) \xi^a \right) T_{ab} \xi^c.
$$

(12.13)

Since $2T_{ab} \xi^a \xi^b = 1$, we have $T_{ab} \xi^a \xi^b = -T_{ab} \xi^a \xi^b$. Likewise $\xi^a \xi_a = -\xi^a \xi_a$. Thus for the first and third terms in (12.13) we can write

$$
T_{ab} \xi^a \xi^b - \xi^c \xi_a T_{ab} \xi^a \xi^b = -T_{ab} \xi^a \xi^b,
$$

(12.14)

which, by Proposition 6, is constant along the Schrödinger trajectory. As a consequence of the Hermitian condition on $T_{ab}$, we find that

$$
\tilde{T}_{ab} \xi^a \xi^b = \tilde{H}^a c \tilde{T}_{ab} \tilde{H}^b d c \xi^d = \{\tilde{T}, \tilde{H}^2\}_\xi,
$$

(12.15)

where $\{\tilde{T}, \tilde{H}^2\}$ is the anticommutator of $\tilde{T}$ and $\tilde{H}^2$. In deriving the second equality in (12.15) we make use of the identity $TH^2 + H^2 T = 2HT\tilde{H}$, which is valid for canonically conjugate operators. On the other hand, the dynamical equation for $\xi^a$ implies that the expression $T_{ab} \xi^a \xi^b$ appearing in the second term of (12.15) is minus the expectation of the anticommutator of $\tilde{T}$ and $\tilde{H}$. Since $\tilde{T}^a = -H^a c \tilde{H}^b d c \tilde{H}^c$ and $\xi^a = -\tilde{H}^a b c \xi^b$, we find that $\tilde{T}^a \xi^b = \langle \tilde{H}^3\rangle$ and $\xi^a \xi^a = \langle \tilde{H}^2\rangle$. Thus, combining together these various expressions, we obtain:

$$
\frac{(\tilde{T}^a \xi^b \nabla_{\xi a} t)^2}{4\tilde{K}_\xi} = \frac{1}{4\langle \tilde{H}^2\rangle K_\xi} \left( \{\tilde{T}, \tilde{H}^2\}_\xi - \langle \tilde{H}^3\rangle \langle \tilde{T}, \tilde{H}\rangle \right)^2.
$$

(12.16)

Let us turn to the term in (12.7) involving $\xi^{(2)a}$. We find that $T_{ab} \xi^a \xi^b = 0$ and $T_{ab} \xi^a \xi^b = 0$. Since $\tilde{c}_a \xi^a = -\langle \tilde{H}^3\rangle$, the contribution from the $\xi^{(2)a}$ term is thus

$$
\frac{(\tilde{c}_a \xi^b \nabla_{\xi a} t)^2}{4\tilde{K}_\xi} = \frac{1}{4\langle \tilde{H}^2\rangle^2 K_\xi} \left( \frac{\langle \tilde{H}^3\rangle^2}{\langle \tilde{H}^2\rangle^3 K_\xi} \right).
$$

(12.17)

If we omit the terms contributing from (12.16), which depend upon the features of the specific choice of estimator $T$, then by consideration of the terms represented in (12.17) we obtain the following sharpened variance bound for $T_{ab}$ which takes the form of a generalised Heisenberg relation:

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Proposition 13. If $T$ and $H$ are canonically conjugate, then the following bound applies to the product of their variances in the Schrödinger state $\xi^a(t)$:

$$
\langle \tilde{T}^2 \rangle / \langle H^2 \rangle \geq \frac{1}{4} \left( 1 + \frac{\langle \tilde{H}^3 \rangle^2}{\langle H^2 \rangle^3 K_\xi^2} \right).
$$

(12.18)

The inequality (12.18) is expressed in terms of natural statistical ‘invariants’, namely, the skewness $\langle \tilde{H}^3 \rangle / \langle H^2 \rangle^3$ and the curvature $K_\xi^2$. Alternatively, we can write (12.18) directly in terms of the central moments of the Hamiltonian:

$$
\langle \tilde{T}^2 \rangle / \langle H^2 \rangle \geq \frac{1}{4} \left( 1 + \frac{\langle \tilde{H}^4 \rangle^2}{\langle H^4 \rangle \langle H^2 \rangle - \langle H^3 \rangle^2 - \langle H^2 \rangle^3} \right).
$$

(12.19)

The positivity of the denominator in the correction term can be verified directly by noting that this is the squared norm of the state $|\psi\rangle$ defined by

$$
|\psi\rangle = \left( \tilde{H}^2 - \frac{\langle \tilde{H}^3 \rangle}{\langle H^2 \rangle} \tilde{H} - \langle \tilde{H}^2 \rangle \right) |\xi\rangle,
$$

assuming $\langle \xi |\xi\rangle = 1$, which is nonvanishing providing that $\tilde{H}^2 |\xi\rangle$ does not lie in the span of $H |\xi\rangle$ and $|\xi\rangle$. This also follows from the statistical identity noted in connection with formula (5.7).

As a further illustration of the general formalism, we exhibit another, distinct bound on the variance, independent of the specific choice of estimator for the time parameter $t$, that arises naturally when we consider inequalities based on the ‘classical system’ of orthogonal vectors associated with $\xi^a(t)$. This bound can be derived when we examine the third order Bhattacharyya type correction, which is given by $(\tilde{\xi}^{(3)} a \nabla_a \tau)^2 / 4 \tilde{\xi}^{(3) a} \tilde{\xi}^{(3) a}$, where $\tilde{\xi}^{(3) a}$ is the component of $\tilde{\xi}^{(3)}$ orthogonal to $\xi^a$, $\tilde{\xi}^a$ and $\tilde{\xi}^b$. Now we know from Lemma 5 that $\tilde{\xi}^a \xi^a$ is constant along quantum trajectories, so $\tilde{\xi} a \xi_a = 0$. Furthermore, $\tilde{\xi} a \xi_a = -\tilde{\xi} a \xi_a$, so $\tilde{\xi}^{(3) a} \xi_a = 0$. Likewise, since $\tilde{\xi} a \xi_a$ is constant, we have $\tilde{\xi}^{(3) a} \xi_a = 0$. Thus $\tilde{\xi}^{(3) a}$ is automatically orthogonal to $\xi^a$ and $\tilde{\xi}^b$ along quantum trajectories. It follows that

$$
\tilde{\xi}^{(3) a} = \xi^{(3) a} - \left( \tilde{\xi} b \xi c / \xi a \xi c \right) \tilde{\xi}^a.
$$

(12.21)

We are interested in the variance bound obtained by consideration of the first and third terms in (5.5):

$$
\text{Var}_\xi[T] \geq \frac{(\xi a \nabla_a t)^2}{4 \xi b \xi^b} + \frac{(\tilde{\xi}^{(3) a} \nabla_a t)^2}{4 \xi^2 a \xi^{(3) a}}.
$$

(12.22)

Now, $\xi^{(3) a} \nabla_a t = -3 \langle \tilde{H}^2 \rangle$ according to Lemma 3. On the other hand, we have $\xi^{(3) a} \tilde{\xi}^a = -\langle \tilde{H}^4 \rangle$ and $\xi^{(3) a} \xi^{(3) a} = \langle \tilde{H}^6 \rangle$, from which it follows that

$$
\tilde{\xi}^{(3) a} \tilde{\xi}^{(3) a} = \langle \tilde{H}^6 \rangle - \frac{\langle \tilde{H}^4 \rangle^2}{\langle H^2 \rangle}.
$$

(12.23)

Putting these ingredients together, we thus obtain the following correction to the Cramér-Rao lower bound (cf. Brody and Hughston 1996b,c).
Proposition 14. If $T$ and $H$ are canonically conjugate observable variables, then the following inequality holds along the Schrödinger trajectory $\xi^a(t)$ generated by $H$:

$$\langle \hat{T}^2 \rangle \langle \hat{H}^2 \rangle \geq \frac{1}{4} \left( 1 + \frac{(\langle \hat{H}^4 \rangle - 3\langle \hat{H}^2 \rangle^2)}{\langle \hat{H}^6 \rangle \langle \hat{H}^2 \rangle - \langle \hat{H}^4 \rangle^2} \right).$$

(12.24)

This correction is also strictly nonnegative, depends only on the given family of probability distributions determined by $\xi^a(t)$, and is independent of the specific choice of the estimator for time parameter. The fact that the denominator in the correction term is positive follows from the observation that it is given by $\langle \hat{H}^2 \rangle$ times the squared norm of the state $|\psi\rangle$ defined by

$$|\psi\rangle = \left( \hat{H}^3 - \frac{\langle \hat{H}^4 \rangle}{\langle \hat{H}^2 \rangle} \hat{H} \right) |\xi\rangle,$$

(12.25)

where $\langle \xi|\xi \rangle = 1$. It is interesting to note that the numerator in the correction is the square of the fourth cumulant of the distribution, usually denoted $\gamma_2$. The distributions for which $\gamma_2 > 0$ are called leptokurtic, and for $\gamma_2 < 0$ platykurtic. If the distribution is mesokurtic ($\gamma_2 = 0$), then this correction vanishes, and an example of such a distribution is the Gaussian. For applications in quantum mechanics, we normally expect a distribution for $H$ that is not Gaussian, since $H$ is typically bounded from below, so (12.24) will generally give a nontrivial correction. In the case of other canonically conjugate variables, e.g., position and momentum, matters are different, and it is possible that a state can have a Gaussian distribution in these variables, as in the case of coherent states.

In order to obtain some simple examples of the sort of numbers that might arise in connection with these corrections, suppose we assume that we have a physical system for which the energy is not definite, but rather has a known distribution, given by a density function $p(E)$. We shall examine the case when the energy has a gamma distribution, given by the density function of the form

$$p(E) = \frac{\sigma^\gamma}{\Gamma(\gamma)} e^{-E/\sigma} E^{\gamma-1},$$

(12.26)

with $0 \leq E \leq \infty$ and $\sigma, \gamma > 0$. This is to say, we have a large number of independent, identical systems with a prescribed Hamiltonian operator $H_{ab}$ and the Schrödinger state $\xi^a$. Then, by a set of measurements we can determine the distribution of the energy, which is characterised by the density function $p(E)$ given by

$$p(E) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \xi^a \xi_b \exp \left[ i\lambda (H^b_a - E\delta^b_a) \right] d\lambda.$$

(12.27)

For a given probability distribution for the energy, whether a self-adjoint Hamiltonian operator with the corresponding spectral resolution exists, or not, is an open problem which we hope to address elsewhere. Here, instead, we rely on the simple observation that the gamma distribution (12.26) appears quite frequently in statistical studies, and hence it may help to provide an element of intuition as regards the behaviour of the correction terms. In the case of the gamma distribution, the moments are $\langle H^n \rangle = (\gamma + n - 1)!/\sigma^n (\gamma - 1)!$, and for the corresponding lowest relevant central moments we find $\langle \hat{H}^2 \rangle = \gamma/\sigma^2$, $\langle \hat{H}^4 \rangle = 3\gamma(\gamma + 2)/\sigma^4$, and

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\[ \langle \tilde{H}^6 \rangle = 5\gamma (3\gamma^2 + 26\gamma + 24)/\sigma^6. \]

It follows that the correction term in (12.24) is independent of the values of the parameter \( \sigma \). We thus obtain
\[
\langle \tilde{T}^2 \rangle \langle \tilde{H}^2 \rangle \geq \frac{1}{4} \left( 1 + \frac{18}{3\gamma^2 + 47\gamma + 42} \right). \tag{12.28}
\]

In general, for Bhattacharyya style corrections based on the ‘classical system’ of orthogonal vectors, the even order contributions turn out to be dependent upon the choice of the estimator \( T \), while the odd order corrections are manifestly independent of the specific choice of \( T \), and can be expressed entirely in terms of central moments of the conjugate observable \( H \). For example, the fifth order correction can be shown to take the form (Brody and Hughston 1996c)
\[
\tilde{H}^2 [\tilde{H}^8 (\tilde{H}^4 - 3(\tilde{H}^2)^2) + \tilde{H}^6 (8\tilde{H}^4 \tilde{H}^2 - \tilde{H}^6) - 5(\tilde{H}^4)^3] \]
\[
\frac{1}{(\tilde{H}^{10}) (\tilde{H}^6 \tilde{H}^2 - (\tilde{H}^4)^2) + 2\tilde{H}^8 \tilde{H}^6 \tilde{H}^4 - (\tilde{H}^8)^2 \tilde{H}^2 - (\tilde{H}^6)^3} (\tilde{H}^6 \tilde{H}^2 - (\tilde{H}^4)^2). \tag{12.29}
\]

Here we have used the slightly simplified notation \( \tilde{H}^n \) for the \( n \)-th moment of the Hamiltonian about its mean. If we assume that the distribution of the energy is given by a basic exponential distribution with probability density \( p(E) = \sigma \exp(-\sigma E) \), which corresponds to the value \( \gamma = 1 \) for the gamma distribution (12.26), then the corrections (12.24) and (12.29) lead to the following bound, independent of the specific value of \( \sigma \):
\[
\langle \tilde{T}^2 \rangle \langle \tilde{H}^2 \rangle \geq \frac{1}{4} \left( 1 + \frac{9}{46} + \frac{284}{290,027,815} \right). \tag{12.30}
\]

The bounds given by (12.24) and (12.29) are significant inasmuch as they apply even if the odd-order central moments of the Hamiltonian vanish, in which case (12.18) would no longer extend the standard Heisenberg relation.

Throughout the discussion here we have confined the argument to consideration of the time measurement problem. In this case we consider the one-parameter family of states generated by the Hamiltonian. However, the same line of argument will apply for other pairs of canonically conjugate observables, such as position and momentum.

The results indicated here can be pursued further in other ways as well, allowing us to consider various examples of natural statistical submanifolds of the quantum state space. For example, in a quantum field theoretic context it is natural to examine the coherent state submanifold of a bosonic Fock space. The geometry of this manifold arises when we consider measurements of the ‘classical’ field associated with the POM generated by the family of all coherent states. Another interesting line of investigation intimately related to the arguments considered here concerns the status of thermodynamic states in classical and quantum statistical mechanics (Brody and Hughston 1996d, 1997a,b).

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References

Accardi, L. and Watson, G.S. (1994), “Quantum Probability and Statistics” unpublished working paper, Princeton University.

Amari, S. (1982), Ann. Statist. 10, 357.

Amari, S. (1985), Differential-Geometrical Methods in Statistics (Springer-Verlag, Berlin).

Anandan, J. and Aharonov, Y. (1990), Phys. Rev. Lett. 65, 1697.

Ashter, A. and Schilling, T.A. (1995), “Geometry of Quantum Mechanics” CAM-94 Physics Meeting, in AIP Conf. Proc. 342, 471, ed. Zapeda, A. (AIP Press, Woodbury, New York).

Barndorff-Nielsen, O.E., Cox, D.R., and Reid, N. (1986), Int. Stat. Rev. 54, 83.

Bhattacharyya, A. (1942), Proc. Sc. Cong.

Bhattacharyya, A. (1946), Sankhyā 8, 1.

Bhattacharyya, A. (1947), Sankhyā 8, 201.

Bhattacharyya, A. (1948), Sankhyā 8, 315.

Bogolubov, N.N., Logunov, A.A., and Todorov, I.T. (1975), Introduction to Axiomatic Quantum Field Theory (W.A. Benjamin, Massachusetts).

Brody, D.C. and Hughston, L.P. (1996a), Phys. Rev. Lett. 77, 2581.

Brody, D.C. and Hughston, L.P. (1996b), “Geometric Models for Quantum Statistical Inference”, in Geometric Issues in the Foundations of Science, volume in honour of Roger Penrose, eds. Huggett, S.A., et al. (OUP, Oxford 1997).

Brody, D.C. and Hughston, L.P. (1996c), Phys. Lett. A (in press).

Brody, D.C. and Hughston, L.P. (1996d), “Geometry of Thermodynamic States”, University of Cambridge Preprint DAMTP 96-112.

Brody, D.C. and Hughston, L.P. (1997a), “Geometrisation of Statistical Mechanics”, University of Cambridge Preprint DAMTP 97-94.

Brody, D.C. and Hughston, L.P. (1997b), “The Quantum Canonical Ensemble”, University of Cambridge Preprint DAMTP 97-103.

Brody, D. and Meister, B. (1996a), Phys. Rev. Lett. 76, 1.

Brody, D. and Meister, B. (1996b), Physica A 223, 348.

Brody, D. and Rivier, N. (1995), Phys. Rev. E 51, 1006.

Burbea, J. (1986), Expo. Math. 4, 347.

Efрон, B. (1975), Ann. Statist. 3, 1189.

Davies, E.B. and Lewis, J.T. (1970), Commun. Math. Phys. 17, 239.

Dawid, A.P. (1975), Ann. Statist. 3, 1231.

Dawid, A.P. (1977), Ann. Statist. 5, 1249.

Field, T.R. (1996), The Quantum Complex Structure, D.Phil. Thesis, Oxford University.

Geroch, R. (1971a), Special Topics in Particle Physics, unpublished lecture notes, University of Texas at Austin.

Geroch, R. (1971b), Ann. Phys. 62, 582.

Gibbons, G.W. (1992), Journ. Geom. Phys. 8, 147.

Gibbons, G.W. and Pohle, H.J. (1993), Nucl. Phys. B410, 117.

Helstrom, C.W. (1969), Journ. Statist. Phys., 1, 231.

Helstrom, C.W. (1976), Quantum Detection and Estimation Theory (Academic Press, New York).

Holevo, A.S. (1973), Journ. Multivariate Anal. 3, 337.

Holevo, A.S. (1979), Rep. Math. Phys. 16, 385.

Holevo, A.S. (1982), Probabilistic and Statistical Aspects of Quantum Theory (North-Holland Publishing Company, Amsterdam).

Hughston, L.P. (1995), “Geometric Aspects of Quantum Mechanics” in Twistor Theory, ed. Huggett, S. (Marcel Dekker, Inc., New York).

Phil. Trans. R. Soc. Lond. A (1996)
Hughston, L.P. (1996), Proc. Roy. Soc. London 452, 953.
Ingarden, R.S. (1981), Int. Journ. Eng. Sci. 19, 1609.
Isham, C.J. (1995), Lectures on Quantum Theory, (Imperial College Press, London).
Jones, K.R.W. (1994), Phys. Rev. A 50, 3682.
Kass, R.E. (1989), Statist. Sci. 4, 188.
Kibble, T.W.B. (1978), Commun. Math. Phys. 64, 73.
Kibble, T.W.B. (1979), Commun. Math. Phys. 65, 189.
Malley, J.D. and Hornstein, J. (1993), Statist. Sci. 8, 433.
Murray, M.K. and Rice, J.W. (1994), Differential Geometry and Statistics (Chapman and Hall, London).
Nagaoka, H. (1994), “Two Quantum Analogues of the Large Deviation Cramér-Rao Inequality”, in IEEE International Symposium on Information Theory.
Penrose, R. and Rindler, W. (1984), Spinors and Space-Time Vol. I (CUP, Cambridge).
Penrose, R. and Rindler, W. (1986), Spinors and Space-Time Vol. II (CUP, Cambridge).
Rao, C.R. (1945), Bull. Calcutta Math. Soc. 37, 81.
Reed, M. and Simon, B. (1974), Methods of Modern Mathematical Physics, I. Functional Analysis (Academic Press, New York).
Segal, I.E. (1947), Ann. Math. 48, 930.
Streater, R.F. (1995), Statistical Dynamics (Imperial College Press, London).
Streater, R.F. (1996), “Statistical Dynamics and Information Geometry”, in Geometrical Methods in Physics, eds. Combe, P. and Nencka, H., (Amer. Math. Soc.).
Stuart, A. and Ord, J.K. (1994), Kendall’s Advanced Theory of Statistics (Oxford University Press, Oxford).
Schilling, T.A. (1996), Geometry of Quantum Mechanics, Ph.D. Thesis, Pennsylvania State University.
Wald, R.M. (1976), Phys. Rev. D 13, 3176.
Wald, R.M. (1994), Quantum Field Theory in Curved Spacetime and Black Hole Thermodynamics (Chicago Univ. Press, Chicago).
Yuen, H.P., Kennedy, R.S., and Lax, M. (1975), IEEE Trans. Inf. Theory, IT-21, 125.