Preparation and Measurement Uncertainty in Quantum Mechanics

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Abstract

This thesis addresses two forms of quantum uncertainty. In part I, we focus on preparation uncertainty, an expression of the fact that there are sets of observables for which the induced probability distributions are not simultaneously sharp in any state. We exactly characterise the preparation uncertainty regions for several finite dimensional case studies, including a new derivation of the preparation uncertainty region for the Pauli observables of qubits, and two qutrit case studies which have not previously been addressed in the literature.

We also consider the variance based preparation uncertainty for position and momentum observables for the well known "particle in a box" system. We see that the appropriate momentum observable is *not* given by the spectral measure of a self-adjoint operator, although the position observable is. The box system lacks the phase-space symmetry used to determine the free particle and particle on a ring systems so determining the box uncertainty region is rather more difficult than in these cases. We give upper and lower bounds on the boundary of the uncertainty region, and show that our upper bound is exact in an interval.

In part II we turn our attention to measurement uncertainty, exploring the space of compatible joint approximations to incompatible target observables. We prove a general theorem, which shows that, for a broad class of figures of merit, the optimal compatible approximations to covariant targets are themselves covariant. This substantially simplifies the problem of determining measurement uncertainty regions for covariant observables, since the space of covariant compatible approximations is smaller than the space of all compatible approximations.

We employ this theorem to derive measurement uncertainty regions for three mutually orthogonal Pauli observables, and for the quantum Fourier pair acting in any finite dimension.

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Acknowledgements and Dedication

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This thesis is dedicated to the memory of Professor Paul Busch, who I am privileged to have called a mentor, and honoured to have called a friend.

I will not be your last student.

Author's declaration

I declare that the work presented in this thesis is original and my own, except where indicated by specific reference in the text, and that I am the sole author. The work was carried out under the supervision of Paul Busch and Roger Colbeck and has not been presented for any other academic award.

Chapter 2 contains background information, and is referenced as such. Chapter 3 is based on research done in collaboration with Paul Busch, and released as reference [19]. Chapter 4 is based on research done in collaboration with Jukka Kiukas. The material in chapter 5 is my own, influenced by discussions with Paul Busch, and is released in reference [66].

List of publications and preprints

- *Introduction to UniversalQCompiler*,
  R. Iten, O. Reardon-Smith, L. Mondada, E. Redmond, R. S. Kohli, R. Colbeck,
  2019, preprint: [arXiv:quant-ph/1904.01072]

- *On Quantum Uncertainty Relations and Uncertainty Regions*,
  P. Busch, O. Reardon-Smith,
  2019, preprint: [arXiv:quant-ph/1901.03695]

- *Simplifying measurement uncertainty with quantum symmetries*,
  O. Reardon-Smith,
  2019, preprint: [arXiv:quant-ph/1909.05055]

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Introduction and Synopsis

In his seminal paper **92** years ago Heisenberg brought attention to two different, but comple-
mentary, forms of uncertainty in quantum mechanics [41]. The first, known as *preparation
uncertainty*, refers to the fact that there exist sets of observables for which there are no states
which make the probability distributions given by the Born rule simultaneously deterministic
for every observable in the set. The standard description of uncertainty (see, for example [33])
in textbooks of quantum mechanics follows this approach, generally focusing on the standard
deviation as a measure of the spread of a probability distribution, and exploring a tradeoff
forcing one standard deviation to become large as another becomes small. This idea has been
explored and generalised extensively in the literature, for example by using different definitions
of the spread of a probability measure [55, 60, 18]. We will explore further generalisations of
this idea in the first part of this thesis.

In recent years it has become well known that the most famous thought experiment in
Heisenberg's 1927 paper does not fit into this preparation focused view of uncertainty, and a
new perspective has emerged known as *measurement uncertainty* [16, 17, 89]. A feature that
separates quantum theory from classical is that quantum theory contains sets of observables
for which there does not exist any joint observable. Such observables are called *incompatible*
and the study of quantum incompatibility is a burgeoning field [39, 20, 38, 65]. On the
other hand it is possible, for example, to form approximations to the original observables
by mixing them with trivial observables[1], and at some level of mixing these approximations
will become compatible [6]. We might broaden this view by considering arbitrary sets of
compatible observables as approximators and, armed with some measure of the goodness of
our approximations, investigate how closely we can approximate the original set.

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[1]Those for which the Born rule probability distribution is independent of the state.

Chapter 3

Here we investigate the concept of an uncertainty region, a slight generalisation of the usual concept of an uncertainty relation. We determine the variance-uncertainty region for all pairs, and an infinite family of triples of sharp ±1 valued observables. These case have been characterised in the literature [52, 1], but we present new derivations, with a geometrical flavour. We also investigate the uncertainty regions of some qutrit systems, where the structure of states is more complex, and analytical bounds are more difficult to obtain. We determine the uncertainty region for a pair obtained by embedding two mutually unbiased qubit observables in a qutrit system, and that for a pair of Gell-Mann observables. We show that the uncertainty region for a pair of Pauli observables is entirely characterised by the Schrödinger uncertainty relation. On the other hand we demonstrate that the Schrödinger relation is insufficient to determine the uncertainty region for Gell-Mann observables.

Chapter 4

Here we consider the preparation uncertainty for "position" and "momentum" observables associated with a standard example system, the so-called "particle in a box" system. The case of the free particle was addressed by Heisenberg and is well known, and uncertainty region for the particle on a ring was characterised by Busch, Kiukas and Werner [13], but the box case does not seem to have been addressed in the literature. We show that it is necessary for the position representation wave-function to vanish at the boundary in order that the momentum variance is finite, although this assumption is often imposed due to the model that the walls of the box are infinite potential barriers. We obtain upper and lower bounds for the boundary curve of the uncertainty region of the particle in a box, and show that our upper bound is tight for an interval comprising slightly under two thirds[2] of the possible position variance values.

Chapter 5

We formulate symmetries of quantum observables via a finite group, with action on the outcome set, and unital, linear representation acting on the effect space. We introduce a systematic approach for exploiting such symmetries via an "invariant mean" map, acting as a projection from the space of quantum observables to the subspace of covariant observables. We show that the "invariant" mean preserves compatibility of observables. Explicitly, a joint observable for the invariant means is given by the invariant mean of the Cartesian joint of the original observables. We apply this to show that for a wide range of figures of merit, the optimal compatible approximations to covariant observables are given by covariant observables. This

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[2]More precisely $1 - \sqrt{\frac{1}{3} - \frac{2}{\pi^2}} \approx 0.64$.

simplifies the problem of characterising measurement uncertainty regions for compatible targets because the set of covariant compatible approximators is smaller than the set of all compatible approximators. We apply this framework to the measurement uncertainty region of three mutually unbiased Pauli observables, and that of the quantum Fourier pair in an arbitrary, finite dimensional space. Unknown to, and independently of, us this latter case was recently addressed by Werner [90] although his methods are rather different from ours, and specific to phase space observables.

We conjecture that the invariant mean map so defined may be generalised to the case of a compact Hausdorff topological group acting on a separable, locally compact metric space, where the average over group elements is replaced by an integral with respect to the Haar measure. Under the additional assumption that the observable that map is applied to is absolutely continuous with respect to a covariant observable.

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Preliminaries

2.1 Mathematical background of quantum theory

2.1.1 Hilbert space theory

We will be considering separable Hilbert spaces over the complex numbers, where separability is taken to mean the existence of a countable orthonormal basis. We will adopt the convention that the inner product, denoted $\langle \cdot | \cdot \rangle$, is linear in the second argument and conjugate-linear in the first. Such an inner product naturally induces a norm $\|\boldsymbol{x}\| := \sqrt{\langle \boldsymbol{x} | \boldsymbol{x} \rangle}$. We will use the notation $\mathscr{L}(V, W)$ for the space of continuous (and equivalently bounded) linear maps between normed vector spaces V and W, over the same field, omitting the second argument if the two spaces are the same. This set is once more a vector space over the same field, with addition and scalar multiplication being defined pointwise. Moreover it inherits a natural norm, called the *operator norm*

$$(2.1.1) \qquad \|\cdot\| : \mathscr{L}(V, W) \to \mathbb{K}$$

$$(2.1.2) \qquad \|T\| := \sup_{\substack{\boldsymbol{v} \in V \\ \|\boldsymbol{v}\| \leq 1}} \|T\boldsymbol{v}\|,$$

under which it is a Banach space. A particularly important special case is the space of maps $\mathscr{L}(V, \mathbb{K})$, where $\mathbb{K}$ is the field underlying V, which we will denote V^*, and is commonly called the topological dual of V. A celebrated theorem due to Riesz [69] and Fréchet [31], commonly called the Riesz representation theorem, states that Hilbert space over $\mathbb{R}$ is isomorphic to its topological dual, and one over $\mathbb{C}$ is anti-isomorphic to its dual. More explicitly every continuous linear functional on a Hilbert space is of the form $\Psi_{\boldsymbol{w}} : \boldsymbol{v} \mapsto \langle \boldsymbol{w} | \boldsymbol{v} \rangle$, for some fixed $\boldsymbol{w} \in V$, and the map $\Psi_{\boldsymbol{w}}$, defined in this way is a continuous linear functional for every $\boldsymbol{w} \in V$.

We are often required to consider maps which are not defined on the whole Hilbert space. An *operator* is a linear map A whose domain, denoted $D(A)$, is a vector subspace (not necessarily closed) of the Hilbert space of interest. A motivating example is the differential operator $\mathbf{P} : \phi \mapsto -i\phi'$, defined on the subspace of absolutely continuous functions in $L^2(\mathbb{R})$, whose weak derivatives are also in $L^2(\mathbb{R})$. If $A : \mathcal{H} \to \mathcal{K}$ is an operator, defined on a dense domain $D(A) \subseteq \mathcal{H}$ we may define the domain of the *adjoint* $D(A^*)$, to be the set of vectors $\psi \in \mathcal{K}$ for which there exists an $\eta_\psi \in \mathcal{H}$ such that

$$(2.1.3) \qquad\qquad \langle \psi | A\phi \rangle = \langle \eta_\psi | \phi \rangle,$$

holds for all $\phi \in D(A)$. We then define A^* on this domain to be

$$(2.1.4) \qquad\qquad A^* \psi = \eta_\psi,$$

noting that the density of $D(A)$ ensures that the element η_ψ is unique, for those ψ for which it exists. For $\mathscr{L}(\mathcal{H})$ the situation is somewhat simpler, the domain of A and A^* can both be taken to be $\mathcal{H}$. In this case the map $A \mapsto A^*$ is a conjugate linear isomorphism preserving the operator norm (2.1.2), and the equations

$$(2.1.5) \qquad\qquad (AB)^* = B^* A^*$$

$$(2.1.6) \qquad\qquad A^{**} = A$$

$$(2.1.7) \qquad\qquad \left(A^{-1}\right)^* = \left(A^*\right)^{-1},$$

hold, with the last equation requiring the additional assumption that A is invertible with bounded inverse.

The *compact operators* are an important subclass of the bounded operators, they are those which may be written as the limit of a sequence of finite rank operators

$$(2.1.8) \qquad\qquad T_n : \varphi \mapsto \sum_{k=0}^{n} \lambda_k \langle f_k | \varphi \rangle | g_k \rangle$$

$$(2.1.9) \qquad\qquad T_n \xrightarrow{n \to \infty} T,$$

where the limit converges in the operator norm and $(f_k)_{k \in \mathbb{N}}$ and $(g_k)_{k \in \mathbb{N}}$ are orthonormal sets in $\mathcal{H}$.

Certain operators are equal to their own adjoint, we call those *self-adjoint*, denoted $\mathscr{L}_s(\mathcal{H})$, and note that they form a vector space over the reals, where the domain of a sum of two operators is the intersection of the domains.

Those operators which may be written in the form $A = B^* B$, for some operator B are called positive, we denote this with $A \geq 0$. The set of such operators forms a *convex cone* in $\mathscr{L}_s(\mathcal{H})$ (see section 2.2, for definitions related to convexity) denoted $\mathscr{L}_s^+(\mathcal{H})$. For any $\psi \in D(A^* A)$ we have that

$$(2.1.10) \qquad\qquad \langle \psi | B^* B \psi \rangle = \langle B\psi | B\psi \rangle$$

$$(2.1.11) \qquad\qquad\qquad = \left\| B\psi \right\|^2 \geq 0.$$

There is a natural a partial order on the space $\mathscr{L}_s(\mathscr{H})$: defined via $\mathscr{L}_s^+(\mathscr{H})$, we will say $A \geq B$, iff $A - B \geq 0$. Every positive operator A has a square root, the unique positive operator B such that $A = B^2$; this may be shown via the spectral theorem, although independent proofs also exist.

We define the operator absolute value to be

$$(2.1.12) \qquad\qquad |A| := \sqrt{A^*A},$$

noting that A^*A and $|A|$ are bounded if and only if A is.

If $(e_k)_{k \in \mathbb{N}}$ is an orthonormal basis for a Hilbert space $\mathscr{H}$ then we define the trace of an operator $A \in \mathscr{L}(\mathscr{H})$ by

$$(2.1.13) \qquad\qquad \operatorname{tr}(A) = \sum_k \langle e_k | A e_k \rangle,$$

however this quantity is not, in general, independent of the basis chosen, even if it is finite, see appendix A.1 for an example. We consider the restricted class of operators such that

$$(2.1.14) \qquad\qquad \sum_k \langle e_k | (|A| e_k) \rangle,$$

converges to some real number for any, equivalently every, basis $(e_k)_{k \in \mathbb{N}}$. We call these operators *trace-class*, denoted $\mathscr{T}(\mathscr{H})$. For elements of $\mathscr{T}(\mathscr{H})$ the infinite sum

$$(2.1.15) \qquad\qquad \operatorname{tr}(A) = \sum_k \langle e_k | A e_k \rangle,$$

is *absolutely convergent*, and is independent of the choice of basis. Every trace-class operator is bounded, and compact. The trace-class operators form a vector space over $\mathbb{C}$, we summarise several useful properties in Lemma 2.1.

Lemma 2.1 (Properties of the trace-class).

- *the trace is a linear functional on $\mathscr{T}(\mathscr{H})$,*

- *the map $(A, B) \mapsto \operatorname{tr}(A^*B)$ is an inner product on $\mathscr{T}(\mathscr{H})$,*

- *the map $A \mapsto \sqrt{\operatorname{tr}(A^*A)}$ is a norm on $\mathscr{T}(\mathscr{H})$, called the Hilbert-Schmidt norm and denoted $\|A\|_{HS}$,*

- $\operatorname{tr}(A^*) = \operatorname{tr}(A)^*$,

- *if A is trace-class and B is bounded then AB and BA are trace-class, hence $\mathscr{T}(\mathscr{H})$ is a two-sided ideal in the bounded operators,*

- *further, the vector-space of maps on the trace-class of the form $A \mapsto \operatorname{tr}(AB)$, where B is bounded is the topological dual of the trace-class.*

Given two Hilbert spaces $\mathscr{H}$ and $\mathscr{K}$ there is a Hilbert space $\mathscr{H}_\otimes$ and a bilinear map $f : \mathscr{H} \times \mathscr{K} \to \mathscr{H}_\otimes$ such that the subspace $\mathbf{span}\left(\{f(\phi,\psi) \,\big|\, \phi \in \mathscr{H}, \psi \in \mathscr{K}\}\right)$ is dense in $\mathscr{H}_\otimes$ and $\langle f(\phi_1,\psi_2)|f(\phi_2,\psi_2)\rangle = \langle \phi_1|\phi_2\rangle\langle \psi_1|\psi_2\rangle$ for all $\phi_1,\phi_2 \in \mathscr{H}$ and $\psi_1,\psi_2 \in \mathscr{K}$. We write $\mathscr{H}_\otimes =: \mathscr{H} \otimes \mathscr{K}$, called the *tensor product* of $\mathscr{H}$ and $\mathscr{K}$, since it is unique up to isomorphism. Given $S \in \mathscr{L}(\mathscr{H})$ and $V \in \mathscr{L}(\mathscr{K})$ there exists a unique operator, $S \otimes T \in \mathscr{L}(\mathscr{H} \otimes \mathscr{K})$ such that

$$(2.1.16) \qquad\qquad (S \otimes T)(\phi \otimes \psi) = (S\phi) \otimes (T\psi),$$

holds for all $\phi \in \mathscr{H}$ and $\psi \in \mathscr{K}$. We call $(S \otimes T)$ the tensor product of S and T and note some fundamental properties in lemma 2.2.

Lemma 2.2 (Properties of the operator tensor product)**.**

- $\alpha(S \otimes T) = (\alpha S) \otimes T = S \otimes (\alpha T)$, *for all $\alpha \in \mathbb{C}$,*

- $(S_1 + S_2) \otimes T = S_1 \otimes T + S_2 \otimes T$,

- $(S_1 \otimes T_1)(S_2 \otimes T_2) = S_1 S_2 \otimes T_1 T_2$,

- $(S \otimes T)^* = S^* \otimes T^*$,

- *if S and T are both self-adjoint, unitary, positive or trace-class then so is $S \otimes T$ respectively,*

- $\mathrm{tr}\,(S \otimes T) = \mathrm{tr}\,(S)\mathrm{tr}\,(T)$.

A partial inverse of the tensor product is the so-called *partial trace*: if $T \in \mathscr{T}(\mathscr{H} \otimes \mathscr{K})$ then there is a unique $T_1 \in \mathscr{T}(\mathscr{H})$ such that

$$(2.1.17) \qquad\qquad \mathrm{tr}\,(T_1 A) = \mathrm{tr}\,(T(A \otimes \mathrm{I}_{\mathscr{K}})),$$

holds for all $A \in \mathscr{L}(\mathscr{H})$. The partial trace is linear, and trace-preserving. It is also positive, in the sense that it maps positive operators to positive operators and completely positive in the sense of definition 2.1.2.

Definition 2.1.1. A subset $\mathscr{A}$ of the algebra of bounded operators on a Hilbert space is a C^*-algebra if it is

- Closed under the operator product $a,b \in \mathscr{A} \implies ab \in \mathscr{A}$,

- Closed under the operator sum $a,b \in \mathscr{A} \implies a + b \in \mathscr{A}$

- Closed under multiplication by complex numbers $a \in \mathscr{A}, \alpha \in \mathbb{C} \implies \alpha a \in \mathscr{A}$

- Closed under taking adjoints: $a \in \mathscr{A} \implies a^* \in \mathscr{A}$

- Closed in the topology induced by the operator norm

We note that this definition is somewhat nonstandard, a C^*-algebra may also be defined as an abstract algebra obeying certain assumptions. However the Gelfand-Naimark theorem [32] shows that all abstract C^*-algebras are isometrically $*$-isomorphic to some C^*-subalgebra of the bounded operators on a Hilbert space. There is, therefore, no loss of generality in taking definition 2.1.1.

Definition 2.1.2. A map $\Phi : \mathscr{A} \to \mathscr{L}(\mathscr{K})$, where $\mathscr{A} \subseteq \mathscr{L}(\mathscr{H})$ is a C^*-algebra is k-positive if the induced map

$$(2.1.18) \qquad \mathrm{id}_k \otimes \Phi : \mathbb{C}^{k \times k} \otimes \mathscr{A} \to \mathbb{C}^{k \times k} \otimes \mathscr{L}(\mathscr{K})$$

is positive, and Φ is *completely positive* if it is k-positive for all $k \in \mathbb{N}$.

Theorem 2.1 (Stinespring). *Let $\Phi : A \to \mathscr{L}(\mathscr{K})$ be a completely positive map, where $A \subseteq \mathscr{L}(\mathscr{H})$ is a C^* algebra, then Φ is completely positive if and only if it admits the representation*

$$(2.1.19) \qquad \Phi(X) = V^* \pi(X) V,$$

where $V : \mathscr{K} \to \mathscr{K}'$ is a a bounded linear map, $\mathscr{K}'$ is a Hilbert space and π is a $*$-homomorphism[1] of A in $\mathscr{L}(\tilde{\mathscr{K}})$.

Of particular interest for applications in quantum theory are the completely positive maps between spaces of trace-class operators which preserve the trace. Recalling that the dual of the trace-class is the space of bounded operators we can define the dual of a trace-preserving completely positive map by requiring that

$$(2.1.20) \qquad \mathrm{tr}\left(A\Phi(B)\right) = \mathrm{tr}\left(\Phi^*(A)B\right),$$

for all $A \in \mathscr{L}(\mathscr{H})$ and $B \in \mathscr{T}(\mathscr{H})$. The dual of a trace-preserving completely positive map is again completely positive and is *unital* $\Phi^*(\mathrm{I}) = \mathrm{I}$ and *normal* in the sense that

$$(2.1.21) \qquad X_a \uparrow X \implies \Phi^*(X_a) \uparrow \Phi(X),$$

where $\uparrow$ denotes the increasing limit. For detailed information on Stinespring's theorem and the properties of positive and completely positive maps see e.g. [80] and [79].

2.1.2 Measures and operator valued measures

Let Ω be a set and $\mathscr{F}$ a subset of the power set of Ω which includes the empty set, is closed under complements and is closed under countable unions. A set with these properties is called a *σ-algebra* on Ω, and an ordered pair $(\Omega, \mathscr{F})$ of set and σ-algebra of subsets is called a *measurable space*. A (positive, extended real) *measure* on $(\Omega, \mathscr{F})$ is a function μ from $\mathscr{F}$ to $\mathbb{R} \cup \{\infty\}$ such that

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[1]A homomorphism of algebras, each equipped with an involution $*$, such that $\pi(a^*) = \pi(a)^*$.

- $\forall S \in \mathscr{F}$, $\mu(S) \geq 0$,

- There exists a set $S \in \mathscr{F}$ such that $\mu(S) \in \mathbb{R}$,

- If $(S_k)_{k \in \mathbb{N}}$ is a countable sequence of non-intersecting sets in $\mathscr{F}$, then $\mu(\bigcup_k S_k) = \sum_k \mu(S_k)$,

From these properties it immediately follows that $\mu(\varnothing) = 0$, as $\mu(S) = \mu(S \cup \varnothing \cup \varnothing \ldots) = \mu(S) + \mu(\varnothing) + \mu(\varnothing) \ldots$. We define general extended real, and complex measures in the obvious way: an extended real measure μ is a pair of positive measures $\mu_\pm$ such that $\mu(S) = \mu_+(S) - \mu_-(S)$, and a complex measure may be defined by its real and imaginary parts. A positive measure such that $\mu(\Omega) = 1$ is called a probability measure, and we denote the set of probability measures on $(\Omega, \mathscr{F})$ by $\mathscr{P}(\Omega, \mathscr{F})$. If Ω has a topology τ then the Borel σ-algebra, denoted $\mathscr{B}(\Omega, \tau)$, or $\mathscr{B}(\Omega)$, where there is no possibility of confusion, is the smallest σ-algebra containing the open sets of τ. The elements of $\mathscr{B}(\Omega)$ are called the Borel sets. All of the probability measures we encounter in this thesis will be Borel, either with respect to the standard topology on the reals or the topology generated by the singleton sets where Ω is finite.

It is essential for the development of the spectral theory of self adjoint operators to consider "measures" which map into (subsets of) the bounded operators on some Hilbert space.

Definition 2.1.3 (Positive operator valued measure). A positive operator valued measure (POVM) on a set Ω with σ-algebra $\mathscr{F}$ is a function $E : \mathscr{F} \to \mathscr{L}_s^+(\mathscr{H})$ such that $E(\Omega) = \mathrm{I}$ and for all sequences of non-intersecting sets in $\mathscr{F}$ $(S_k)_{k \in \mathbb{N}}$ we have

$$(2.1.22) \qquad E\left(\bigcup_k S_k\right) = \sum_k E(S_k).$$

We note that one can show that the effects (often called POVM elements) $\{E(S) | S \in \mathscr{F}\}$ are bounded operators, in particular $\|E(S)\varphi\| \leq \|E(\Omega)\varphi\| = \|\varphi\|$. We will often be interested in the case where a POVM is a projection valued measure (PVM), in the sense that $E(S)^2 = E(S)$, for all $S \in \mathscr{F}$. Equivalent to this definition is a multiplicative property $E(S)E(T) = E(S \cap T)$, for all $S, T \in \mathscr{F}$. Given a Borel PVM E_A over the reals, there is a vector subspace $D(A) \subseteq \mathscr{H}$ such that the integral

$$(2.1.23) \qquad \int_{\mathbb{R}} x \, d\langle \psi | E_A(x) \phi \rangle$$

converges for all $\psi, \phi \in D(A)$, and a unique self-adjoint operator A with domain $D(A)$ such that

$$(2.1.24) \qquad \langle \psi | A\phi \rangle = \int_{\mathbb{R}} x \, dE_a(x),$$

for ψ, ϕ in the domain.

We give several versions of the spectral theorem, the first of which is the converse of the above statement.

Theorem 2.2 (Spectral theorem for self-adjoint operators). *If A is a self-adjoint operator with dense domain $D(A)$, then there is a unique PVM E_A such that*

$$(2.1.25) \qquad \langle \psi | A\phi \rangle = \int_{\mathbb{R}} x \, d \langle \psi | E_A(x)\phi \rangle,$$

holds for all $\psi, \phi \in D(A)$.

Theorem 2.3 (Spectral theorem for self-adjoint operators - bounded functional calculus). *Let A be a self-adjoint operator on $\mathcal{H}$, there is a unique map $\hat{\phi}$ from the bounded Borel functions on $\mathbb{R}$ to $\mathcal{L}(\mathcal{H})$ such that*

- *$\hat{\phi}$ is an algebraic $*$-homomorphism,*

- *$\hat{\phi}$ is norm continuous $\left\| \hat{\phi}(h) \right\| \leq \|h\|_{\infty}$,*

- *if h_n is a sequence of bounded Borel functions converging (pointwise) to the identity function and $|h_n(x)| \leq x$ for all x and n, then for any $\psi \in D(A)$ we have $\lim_{n\to\infty} \hat{\phi}(h_n)\psi = A\psi$,*

- *if $h_n \to h$ pointwise and the sequence $\|h_n\|_{\infty}$ is bounded then $\hat{\phi}(h_n) \to \hat{\phi}(h)$ strongly,*

- *if $A\psi = \lambda\psi$ then $\hat{\phi}(h)\psi = h(\lambda)\psi$,*

- *if $h \geq 0$ then $\hat{\phi}(h) \geq 0$.*

We use this as a stepping stone to a more general formulation.

Theorem 2.4 (Spectral theorem for self-adjoint operators - Borel functional calculus). *Let A be a self-adjoint operator on $\mathcal{H}$, and χ_{Ω} the characteristic function of the measurable set $\Omega \subseteq \mathbb{R}$. We define the operators $P_{\Omega} = \hat{\phi}(\chi_{\Omega})$, and note the properties*

- *the P_{Ω} are orthogonal projections,*

- *$P_{\mathbb{R}} = I$ and $P_{\varnothing} = 0$,*

- *if Ω is a countable union of disjoint sets Ω_n then $P_{\Omega} = \lim_{N\to\infty} \sum_{n=1}^{N} P_{\Omega_n}$, where the limit converges strongly,*

- *$P_{\Omega} P_{\Delta} = P_{\Omega \cap \Delta}$.*

We call the map $E_A : \Omega \mapsto P_{\Omega}$ the spectral measure of A. The map $\Omega \mapsto \langle \psi | P_{\Omega} \phi \rangle$ is a complex-valued Borel measure on $\mathbb{R}$ for each $\psi, \phi \in \mathcal{H}$ and denote it $\mu_{\psi\phi}$. If g is a bounded Borel function on $\mathbb{R}$ then we can define $g(A)$ by

$$(2.1.26) \qquad \langle \psi | g(A)\phi \rangle = \int_{\mathbb{R}} g(\lambda) \, d\mu_{\psi\phi}(\lambda),$$

and note that this agrees with $\hat{\phi}(g)$, further if g is an unbounded, complex valued Borel function on $\mathbb{R}$ we define

$$(2.1.27) \qquad D(g(A)) = \left\{ \psi \,\middle|\, \int_{\mathbb{R}} |g(\lambda)|^2 d\mu_{\psi\psi}(\lambda) < \infty \right\}$$

$$(2.1.28) \qquad \langle \psi | g(A)\phi \rangle = \int_{\mathbb{R}} g(\lambda) d\mu_{\psi\phi}(\lambda).$$

We write $g(A) = \int_{\mathbb{R}} g(\lambda) P_\lambda$, and note that $g(A)$ is self-adjoint if g is real.

We call the support of a self-adjoint operator A, $\mathrm{supp}(A)$, the complement of the union of all the open sets Ω for which $P_\Omega = 0$, and note that we can restrict the integrals over $\mathbb{R}$ in the previous theorem to be over $\mathrm{supp}(A)$; we therefore allow Borel functions defined on $\mathrm{supp}(A)$, rather than requiring that they are defined on the whole real line. We note that the definition of the support given here matches the *spectrum* of a closed operator

$$(2.1.29) \qquad \sigma(A) = \mathbb{C} \setminus \rho(A),$$

where the *resolvant set*, $\rho(A)$ is defined to be the set of $\lambda \in \mathbb{C}$ for which $\lambda I - A$ is a bijection onto $\mathscr{H}$ with a bounded inverse. For a self-adjoint operator the terms spectrum and support are interchangeable.

Some important special cases are: the spectral measure of a compact operator is supported on a finite number of points or a sequence of points which converges to zero; the spectral measure of an operator on a finite dimensional Hilbert space is supported on a finite number of points; the spectral measure of a positive operator is supported within the non-negative real numbers.

2.2 Convex analysis

Convex analysis concerns itself with convex sets and convex functions. Although there is an interesting theory of convex subsets of infinite dimensional vector spaces[2] this is beyond the scope of this thesis. Here all convex sets will be subsets of finite dimensional real vector spaces. We will follow the exposition of Rockafellar [71]. Since we are only dealing with finite dimensional spaces a vector space V is canonically isometrically isomorphic to its bidual V^{**}, and we do not distinguish the two, equating the vector $\boldsymbol{x} \in V$ and the evaluation map $(\psi \mapsto \psi(\boldsymbol{x})) \in V^{**}$. This identification is convenient for discussing the convex conjugate of a function.

Definition 2.2.1. A subset C of a real vector space is *convex* if for all $\boldsymbol{x}, \boldsymbol{y} \in C$ and for all $\lambda \in [0,1]$

$$(2.2.1) \qquad \lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y} \in C.$$

---

[2]See, for example [59].

Examples of convex sets include

- Any interval in $\mathbb{R}$,

- The balls in any normed vector space over the reals,

- The state-space $\mathscr{S}$ of quantum mechanics, defined in Section 2.4,

- The set of points in $\mathbb{R}^2$ that lie "above" the graph of the function $x \mapsto x^2$, i.e. the set of points $\{(x,y) \mid y > x^2\}$.

This last example motivates the definition of a convex function

Definition 2.2.2. The *epigraph* of a function $f : V \to \mathbb{R}$, where V is a real vector space is the set of points in the vector space $V \oplus \mathbb{R}$ "above" the graph of f,

$$\text{(2.2.2)} \qquad \qquad \text{epi}\, f = \left\{ (v, \mu) \,\middle|\, v \in V, \mu \in \mathbb{R}, \mu \geq f(v) \right\}.$$

Definition 2.2.3. A function from a real vector-space to the reals is *convex* if its epigraph is a convex set.

This definition of convexity for functions is slightly too restrictive, in the present context, since it only covers functions defined on an entire vector space V. We will mainly be concerned with, for example, uncertainty measures which are non-negative, and so we are motivated to find a definition of convexity appropriate for more general domains.

It is convenient to define the extended reals $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty, -\infty\}$, with the obvious axioms for extending the order relation, addition and multiplication. We also define $\inf \varnothing = \infty$ and $\sup \varnothing = -\infty$. We can now consider functions defined on arbitrary convex subsets of real vector spaces, simply by extending the function to be ∞ outside. We note that, strictly speaking, this recourse to the extended reals is unnecessary and one can consider convex functions defined on convex subsets of real vector spaces directly, but this leads to more tedious consideration of domains. In the present formulation one can recover the domain by considering the points where the extended function takes finite values. The forms $\infty - \infty$ and $-\infty + \infty$ are left undefined, in principle it is important to be cautious about these cases, but they do not arise within this work.

For completeness we define the epigraph and convexity for extended real functions, although these are essentially identical to definitions given above.

Definition 2.2.4. A function $f : V \to \overline{\mathbb{R}}$, where V is a real vector space, is *convex* if its epigraph

$$\text{(2.2.3)} \qquad \qquad \text{epi}\, f = \left\{ (v, \mu) \,\middle|\, v \in V, \mu \in \mathbb{R}, \mu \geq f(v) \right\},$$

is a convex subset of $V \oplus R$. Note that if $f(v) = \infty$ there are no $\mu \in \mathbb{R}$ such that $\mu \geq f(v)$, so these v do not occur in any of the ordered pairs in $\text{epi}\, f$.

We now state two useful theorems of convex functions.

Theorem 2.5. *Let $f : V \to (-\infty, \infty]$, with V a real vector space. Then f is convex if and only if the inequality*

$$(2.2.4) \qquad f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}) \leq \lambda f(\boldsymbol{x}) + (1-\lambda)f(\boldsymbol{y})$$

holds for all $\boldsymbol{x}, \boldsymbol{y} \in V$ and $\lambda \in [0,1]$. The exception of $-\infty$ is to exclude pathological cases where $f(\boldsymbol{x})$ and $f(\boldsymbol{y})$ are different infinite values.

Theorem 2.6 (Jensen's inequality)**.** *Let $f : V \to (-\infty, \infty]$, with V a real vector space. Then f is convex if and only if the inequality*

$$(2.2.5) \qquad f\left(\sum_{i=1}^{n} \lambda_i \boldsymbol{x}_i\right) \leq \sum_{i=1}^{n} \lambda_i f(\boldsymbol{x}_i),$$

holds for all $\boldsymbol{x}_i \in V$ and $\lambda_i \in [0,1]$ such that $\sum_{i=1}^{n} \lambda_i = 1$.

There are also generalisations to countable sets of points, and probability measures in the uncountable case [25][64].

It is useful to define the *convex conjugate* of a function, which we will apply extensively in section 5.

Definition 2.2.5. Given a function $f : V \to \overline{\mathbb{R}}$, where V is a topological vector space over the reals, we define the convex conjugate of f to be

$$(2.2.6) \qquad f^* : V^* \to \overline{\mathbb{R}}$$
$$(2.2.7) \qquad f^* : \boldsymbol{\alpha} \mapsto \sup_{\boldsymbol{v} \in V}\{\langle \boldsymbol{\alpha}, \boldsymbol{v} \rangle - f(\boldsymbol{v})\},$$

where V^* is the space of continuous linear functionals on V and $\langle \cdot, \cdot \rangle$ denotes the dual pairing between V and V^*.

Theorem 2.7. *The biconjugate $(f^*)^*$ of a function $f : V \to \overline{\mathbb{R}}$ is the greatest (pointwise) lower-semi continuous function which is bounded above by f.*

Where f is a convex function $(f^*)^*$ (hereafter denoted f^{**}) is equal to f.

2.3 Semidefinite programming

The usual formulation [84] of semi-definite programming is in terms of $n \times n$ positive-semidefinite real matrices with real elements. Here, following the exposition given in [87], we use a slightly different but entirely equivalent formulation better adapted to problems in quantum mechanics.

Definition 2.3.1. Let $\mathscr{H}$, $\mathscr{K}$ be finite-dimensional Hilbert spaces, $\mathrm{C} \in \mathscr{L}_s(\mathscr{H})$, $\mathrm{D} \in \mathscr{L}_s(\mathscr{K})$ and let $\Psi : \mathscr{L}_s(\mathscr{H}) \to \mathscr{L}_s(\mathscr{K})$ be a linear map. The *primal semidefinite problem* and *dual semidefinite problem* associated to the triple $(\Psi, \mathrm{C}, \mathrm{D})$ are

(2.3.1)
$$
\begin{array}{llll}
\underset{X \in \mathscr{L}_s^+(\mathscr{H})}{\text{maximise}} & \mathbf{tr}\,(\mathrm{C}X) & \underset{Y \in \mathscr{L}_s^+(\mathscr{K})}{\text{minimise}} & \mathbf{tr}\,(\mathrm{D}Y) \\[2mm]
\text{subject to} & \Psi(X) \le \mathrm{D} & \text{subject to} & \Psi^*(Y) \ge C,
\end{array}
$$

respectively.

Here it is traditional to note the analogy with the classical theory of linear programming, we therefore note the duality theorem for linear programs (2.8) from ref. [72].

Theorem 2.8. *Let* $\mathrm{A} \in \mathbb{R}^{n \times m}$, $\boldsymbol{c} \in \mathbb{R}^n$ *and* $\boldsymbol{b} \in \mathbb{R}^m$ *then*

(2.3.2)
$$
\sup\left\{\boldsymbol{c} \cdot \boldsymbol{x} \,\middle|\, \boldsymbol{x} \in \mathbb{R}^n, A\boldsymbol{x} \le \boldsymbol{b}\right\} = \inf\left\{\boldsymbol{b} \cdot \boldsymbol{y} \,\middle|\, \boldsymbol{y} \in \mathbb{R}^m, A^T \boldsymbol{y} = \boldsymbol{c}\right\},
$$

if at least one of the sets is non-empty, with the convention that the $\sup$ *and* $\inf$ *of an empty set are* $-\infty$ *and* ∞, *respectively.*

The analogy follows from considering the trace of the product of two operators as an inner product on the (real) vector vector space of self-adjoint operators on a given Hilbert space. The extra complication that comes from considering operator inequalities rather than vector inequalities causes the duality theory for semidefinite programs to be somewhat weaker than that for linear programs.

Definition 2.3.2. Given a triple $(\Psi, \mathrm{C}, \mathrm{D})$, chosen as in definition 2.3.1 we define the *primal feasible set* and *dual feasible set* to be

(2.3.3)
$$
\mathscr{P} = \left\{X \in \mathscr{L}_s^+(\mathscr{H}) \,\middle|\, \Psi(X) \le \mathrm{D}\right\}
$$

and

(2.3.4)
$$
\mathscr{D} = \left\{Y \in \mathscr{L}_s^+(\mathscr{K}) \,\middle|\, \Psi^*(Y) \ge \mathrm{C}\right\},
$$

respectively.

Theorem 2.9 (Weak duality)**.** *For every triple* $(\Psi, \mathrm{C}, \mathrm{D})$ *chosen as in definition 2.3.1 the inequality*

(2.3.5)
$$
\sup_{X \in \mathscr{P}} \mathbf{tr}\,(\mathrm{C}X) \le \inf_{Y \in \mathscr{D}} \mathbf{tr}\,(\mathrm{D}Y),
$$

holds.

A proof of theorem 2.9 is contained in ref. [84]. We call a semidefinite problem *strongly dual* if

$$(2.3.6) \qquad\qquad \sup_{X \in \mathscr{P}} \operatorname{tr}(\mathrm{C}X) = \inf_{Y \in \mathscr{D}} \operatorname{tr}(\mathrm{D}Y).$$

Although necessary conditions are not easy to find Slater's condition [78] is sufficient to prove strong duality, and in practice is how such problems are approached.

Theorem 2.10 (Slater's condition)**.** *Let* $(\Psi, \mathrm{C}, \mathrm{D})$ *be chosen as in definition 2.3.1, then the following two implications hold:*

1. *If* $\inf_{Y \in \mathscr{D}} \operatorname{tr}(\mathrm{D}Y) \in \mathbb{R}$ *and there exists an operator* $X > 0$ *such that* $\Psi(X) < \mathrm{D}$, *then the equality* (2.3.6) *holds and there exists an operator* $Y \in \mathscr{D}$ *achieving the infimum.*

2. *If* $\sup_{Y \in \mathscr{P}} \operatorname{tr}(\mathrm{C}X) \in \mathbb{R}$ *and there exists an operator* $Y > 0$ *such that* $\Psi^*(Y) > \mathrm{C}$, *then the equality* (2.3.6) *holds and there exists an operator* $X \in \mathscr{P}$ *achieving the supremum.*

2.4   Quantum theory

Throughout this thesis we will use the standard formulation of quantum mechanics, in the main following the exposition of references [14] and [43]. All Hilbert spaces are assumed to be over the field of complex numbers. The quantum states will be the positive, trace-class operators on $\mathscr{H}$ with trace equal to 1 and will be denoted $\mathscr{S}(\mathscr{H})$. There is a natural convex structure to the states. Given states ρ and σ and a real $\lambda \in [0, 1]$, the convex combinations $\lambda \rho + (1 - \lambda)\sigma$ are also states which may be interpreted as preparing ρ with probability λ and σ with probability $1 - \lambda$. We also allow countable combinations $\sum_{i \in \mathbb{N}} \lambda_i \rho_i$, where $\lambda_i \geq 0$ and $\sum_{i \in \mathbb{N}} \lambda_i = 1$, to be interpreted analogously. There are certain operators which may not be expressed as a convex combination in a non-trivial way, i.e. a decomposition $\rho = \sum_{i \in \mathbb{N}} \lambda_i \rho_i$ requires that $\rho_i \neq \rho \implies \lambda_i = 0$. We call these the *pure* states of quantum theory. An application of the spectral theorem shows that they are given by rank-1 projections and that every quantum state may be written as a countable convex combination of pure states.

We expect the observables of quantum theory to be maps taking a quantum state and returning a probability measure over an outcome set. This matches what happens in experiments where one applies an observable to an input state and gets an output drawn from some probability distribution. It is natural to require that these maps respect the convex structure of the state space, in the sense that if one prepares a probabilistic mixture of states and measures an observable, one expects the probability distribution obtained on the mixture of states to be the mixture of the probability distributions obtained from the original states.

Definition 2.4.1. Let $(\Omega, \mathscr{F})$ be a measure space and $\mathscr{H}$ a Hilbert space. A map $M : \mathscr{S}(\mathscr{H}) \to \mathscr{P}(\Omega, \mathscr{F})$ is *linear* if for all convex combinations of states $\sum_{i \in \mathbb{N}} \lambda_i \rho_i$ we have

$$(2.4.1) \qquad M\left(\sum_{i \in \mathbb{N}} \lambda_i \rho_i\right) = \sum_{i \in \mathbb{N}} \lambda_i M\left(\rho_i\right),$$

where addition and scalar multiplication of measures is defined pointwise.

Maps of this form have a useful representation in terms of positive operator valued measures.

Theorem 2.11. *Let $(\Omega, \mathscr{F})$ be a measure space, $\mathscr{H}$ a Hilbert space and let $M : \mathscr{S}(\mathscr{H}) \to \mathscr{P}(\Omega, \mathscr{F})$ be a linear map, then there exists a POVM $E : \mathscr{F} \to \mathscr{L}_s^+(\mathscr{H})$ such that*

$$(2.4.2) \qquad M(\rho) : X \to \mathrm{tr}\left(E(X)\rho\right).$$

The proof of this theorem is essentially identical to the methods used in [61], although with weaker assumptions on the observables. The converse is also true, each POVM gives rise to a linear map from the state space to the space of probability measures. We denote the probability measure obtained by the pairing between a POVM $\mathbf{E}$ and a state ρ with $\mathbf{E}_\rho : X \mapsto \mathrm{tr}\left(\mathbf{E}(X)\rho\right)$.

We henceforth consider POVMs and linear maps to be interchangeable, and use the term "observable" for both. Where the outcome set Ω is finite and the set of events $\mathscr{A}$ is the entire power set of Ω, a simpler definition suffices. In this case a POVM is defined entirely by its action on the singleton sets, so we can equivalently consider a map $\mathbf{E} : \Omega \to \mathscr{L}_s^+$, such that $\sum_{\omega \in \Omega} \mathbf{E}(\omega) = \mathbf{I}$. We call *sharp* those Borel observables on the real line whose range consists of orthogonal projections. An application of the spectral theorem shows that the sharp observables are the spectral measures of self-adjoint operators. It is sometimes more convenient to consider the self-adjoint operator instead of the POVM, for example, if E is the spectral measure of the bounded operator A then

$$(2.4.3) \qquad \langle E^\rho \rangle = \mathrm{tr}\left(A\rho\right),$$

where the angle brackets denote the mean, or expected value of the probability distribution E^ρ.

Given two quantum observables, say $E_1 : \mathscr{F}_1 \to \mathscr{L}_s^+(\mathscr{H})$ and $E_2 : \mathscr{F}_2 \to \mathscr{L}_s^+$, where $(\Omega_1, \mathscr{F}_1)$ and $(\Omega_2, \mathscr{F}_2)$ are measurable spaces there may exist a joint, an observable J on the product measure space $(\Omega_1 \times \Omega_2, \mathscr{F}_1 \otimes \mathscr{F}_2)$ such that

$$(2.4.4) \qquad J(A \times \Omega_2) = E_1(A), \quad \forall A \in \mathscr{F}_1,$$

$$(2.4.5) \qquad J(\Omega_1 \times A) = E_2(A), \quad \forall A \in \mathscr{F}_2.$$

When such a joint observable exists we call the E_1 and E_2 *compatible*, two observables will generally be incompatible.

(a) A Stern-Gerlach type device correctly measures the $\sigma_{\mathbf{z}}$ observable on some input qubits, each in a $\sigma_{\mathbf{z}}$ eigenstate.

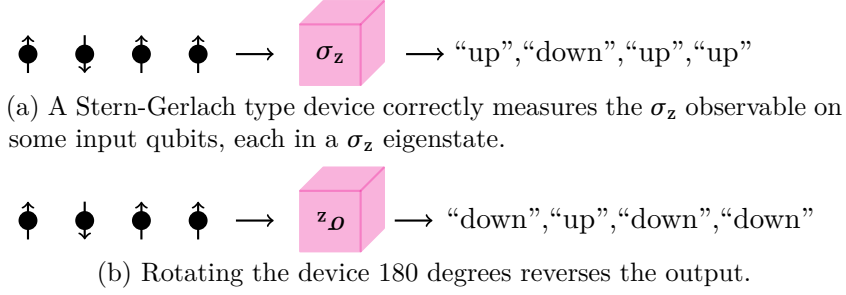(b) Rotating the device 180 degrees reverses the output.

Figure 2.1: The group $\{0, 1\}$ with addition modulo 2, with the group representation implementing "flipping the measuring upside-down", action $f_g : h \mapsto gh$, and the observable $\sigma_{\mathbf{z}}$ form a system of covariance.

Definition 2.4.2. Given a group G, with an action $f_g : \Omega \to \Omega$, $g \in G$, and a representation $\{R_g \mid g \in G\}$ as positive, unital, linear maps acting on $\mathscr{L}_s(\mathscr{H})$, we say that an observable $E : \mathscr{F} \to \mathscr{L}_s(\mathscr{H})$ is $(G, R, f)-covariant$ if

$$(2.4.6) \qquad E(f_g(X)) = R_g[E(X)], \quad \forall g \in G, X \in \mathscr{F}$$

where $\mathscr{F}$ is the σ-algebra of measurable sets over Ω. Where there is no possibility of confusion we will simply call these observables *covariant*.

Note that the R_g must be unital since

$$(2.4.7) \qquad \mathrm{I} = \mathrm{E}(f_g(\Omega)) = R_g[\Omega] = R_g[\mathrm{I}].$$

A group, representation, action and observable satisfying equation (2.4.6) are called a *system of covariance*, where the observable $\mathbf{E}$ is projection-valued this is equivalent to a system of imprimitivity, well known in the representation theory literature (see, e.g. [57], for an introduction). Figure 2.1 describes a simple system of covariance.

An application of Wigner's theorem [94, 93] shows that the representation must be of the form

$$(2.4.8) \qquad R_g : A \mapsto U_g A U_g^*,$$

where the U_g are either unitary or anti-unitary operators on $\mathscr{H}$. Since anti-unitary operators, and anti-linear operators in general, are much less common than their linear counterparts in the quantum information and foundation literature we note the following example, a map $K : \mathbb{C}^n \to \mathbb{C}^n$ provided by fixing an orthonormal basis $B = |0\rangle \dots |n-1\rangle$, and defining

$$(2.4.9) \qquad K : |\varphi\rangle \mapsto \sum_i \langle i|\varphi\rangle^* |i\rangle,$$

which differs from a definition of the identity operator only by the complex conjugate. The resulting map is not, of course, independent of the basis chosen, however, for any two anti-unitary maps K, K' there exists a unitary U such that

$$(2.4.10) \qquad K' = UK,$$

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so a single anti-unitary, combined with the familiar structure of the unitary operators, suffices to explore the space of anti-unitaries [95].

Covariant quantum observables were introduced by Davies [28], using the language of general quantum instruments rather than POVMs, and were already being used in the study of uncertainty by Holevo in 1978 [44]. Special cases which have been studied in the literature are covariant symmetric informationally complete-POVMS (SIC-POVMs) [4, 67] and extreme covariant POVMs [21, 35, 23, 34]. Covariance has been employed in the study of measurement uncertainty for angular momentum observables [27], number and angle [13], and general phase spaces [90].

The time evolution will be given by quantum channels, those linear maps from the trace-class operators on one Hilbert space to the trace-class operators on another which preserve the trace, and are completely positive. A corollary of Stinespring's Theorem 2.1 states that the completely positive maps from a Banach space $\mathcal{U} \subseteq \mathcal{L}(\mathcal{H})$ to $\mathcal{L}(\mathcal{K})$ are exactly those which may be written in the form

$$(2.4.11) \qquad \Phi(\rho) = \operatorname{tr}_{\mathcal{H}_0}\left(U\rho \otimes \rho_0 U^*\right),$$

where $\mathcal{H}_0$ is a Hilbert space and ρ_0 is a quantum state in H_0. One may, alternatively, consider the quantum state to be unchanging and allow the observables to evolve. This "Heisenberg picture" (in contrast to the former "Schrödinger picture") is furnished by the dual map and is sometimes more convenient.

The dynamics of a perfectly isolated quantum system are reversible, using Wigner's theorem it is possible to show that the bijective channels are those of the form

$$(2.4.12) \qquad \Phi : \rho \mapsto U\rho U^*$$

$$(2.4.13) \qquad \Phi^* : E(X) \mapsto U^*E(X)U,$$

where $U : \mathcal{H} \to \mathcal{H}$ is a unitary or anti-unitary map, (see [93] for a translation of the original work [94], or [7] for a detailed proof). The time evolution of quantum mechanics is given by the unitary case, although the anti-unitary operators will be useful in section 5 when we consider observables symmetric under the action of a group with a representation consisting of both unitary and anti-unitary maps.

2.5 Comparing measures and observables

The textbook description of quantum uncertainty (see e.g. [62]) may be summarised as the claim that there exist pairs of quantum observables $\mathbf{E}$, $\mathbf{F}$ for which there does not exist any state ρ which makes the induced probability measures $\mathbf{E}^\rho$ and $\mathbf{F}^\rho$ simultaneously sharply concentrated. Often this is characterised by a lower bound on some functional of the variances or entropies [55, 88] of the two distributions, valid for all quantum states. A slightly broader

view is to consider the set

$$(2.5.1) \qquad \left\{ \left(\delta(\mathbf{E}_1^\rho), ..., \delta(\mathbf{E}_n^\rho) \right) \middle| \rho \in \mathscr{S}(\mathscr{H}) \right\} \subseteq \mathbb{R}^n,$$

where the $\mathbf{E}_i$ are observables on $\mathscr{H}$ and δ is a measure of the uncertainty of a probability measure (e.g. (2.5.30), (2.5.32) or (2.5.49)). This approach is known as *preparation uncertainty*, since we range over the quantum states (also called preparations).

An alternative facet of quantum uncertainty is called *measurement uncertainty*. This is a consequence of the fact that quantum mechanics contains incompatible observables, that is, there exist pairs (or larger collections) of quantum observables for which there is no joint observable. We can make quantitative the qualitative statement that a family of observables is incompatible by considering the distance of each observable from the corresponding margin of an *approximate joint observable*, in more mathematical language, given $\{ E_i : \mathscr{F}_i \to \mathscr{S}(\mathscr{H}) | i \in 1...n \}$, and δ, representing a distance between observables we are interested in the set

$$(2.5.2) \qquad \{ (\delta(E_1, F_1), ..., \delta(E_n, F_n)) | F_i : \mathscr{F}_i \to \mathscr{S}(\mathscr{H}) \text{ are all compatible} \}.$$

Loosely, the E_i are a family of target observables that we would like to measure, incompatibility prohibits this, but we want to know how close we can come to approximating them all simultaneously. This situation is depicted in figure 5.1.

To develop the theory of uncertainty, and particularly measurement uncertainty, it is useful to be able to compare probability measures on some space. For example we might want to make the claim that one distribution is "broader" than another, or that one of two distributions approximates a third, target distribution, more accurately than the other. Here we introduce the mathematical tools we will use to do this.

In section 5 we will compare finite-outcome probability distributions using the L^p-metric, defined as

$$(2.5.3) \qquad \delta_p(S, T) := \left(\sum_{\omega \in \Omega} |S(\omega) - T(\omega)|^p \right)^{\frac{1}{p}}, \quad 1 \leq p < \infty,$$

$$(2.5.4) \qquad \delta_\infty(S, T) := \max_{\omega \in \Omega} |S(\omega) - T(\omega)|.$$

Note here we are considering probability distributions as functions on the outcome set Ω, rather than measures as function on a σ algebra over Ω. The former notation is not well suited to measures with infinite outcome sets, but we will employ it extensively in the finite outcome setting. We note the L^1 metric is equal to the definition of total variation distance given in the standard references, e.g. [85] and [86], which has a natural generalisation to the case of measures with infinite outcomes

$$(2.5.5) \qquad \delta_1(\mu, \nu) := \sup_{S \in \mathscr{F}} |\mu(S) - \nu(S)|.$$

The use of the total variation for measurement errors of continuous variables has been criticised in [17], on the basis that it is insensitive to any metric on the underlying space. Explicitly, every point measure is at distance 2 from every other point measure, whereas in a physical context it is often natural to consider point measures corresponding to points which are close together to be similarly close.

Definition 2.5.1. If (A, d) is a metric space and $\alpha > 0$ then the Wasserstein α-metric is

$$(2.5.6) \qquad W_\alpha\left(\mu, v\right) := \left(\inf_{\gamma \in \Gamma(\mu, v)} \int_{A \times A} d(x, y)^\alpha d\gamma(x, y)\right)^{\frac{1}{\alpha}}.$$

Here $\Gamma(\mu, v)$ is the set of "couplings" between μ and v, the probability measures on the product space $A \times A$, with first margin μ and second margin v.

We provide a simple example, computing the Wasserstein αdistance between two probability distributions on the outcome set $\{-1, 1\}$. We let

$$(2.5.7) \qquad \mu(1) = m$$

$$(2.5.8) \qquad \mu(-1) = 1 - m$$

$$(2.5.9) \qquad v(1) = v$$

$$(2.5.10) \qquad v(-1) = 1 - v.$$

An arbitrary probability distribution on the outcome set $\{-1, 1\} \times \{-1, 1\} = \{(1, 1), (1, -1), (-1, 1), (-1, -1)\}$ is given by

$$(2.5.11) \qquad p(1, 1) = a$$

$$(2.5.12) \qquad p(1, -1) = b$$

$$(2.5.13) \qquad p(-1, 1) = c$$

$$(2.5.14) \qquad p(-1, -1) = 1 - a - b - c.$$

Applying the constraint that p is a coupling of μ and v we obtain

$$(2.5.15) \qquad p(1, 1) + p(1, -1) = a + b = \mu(1) = m$$

$$(2.5.16) \qquad p(-1, 1) + p(-1, -1) = 1 - a - b = \mu(-1) = 1 - m$$

$$(2.5.17) \qquad p(1, 1) + p(-1, 1) = a + c = v(1) = v$$

$$(2.5.18) \qquad p(1, -1) + p(-1, -1) = 1 - a - c = v(-1) = 1 - v.$$

We therefore have a family of couplings parameterised by a single real parameter

$$(2.5.19) \qquad p_a(1, 1) = a$$

$$(2.5.20) \qquad p_a(1, -1) = m - a$$

$$(2.5.21) \qquad p_a(-1, 1) = v - a$$

$$(2.5.22) \qquad p_a(-1, -1) = 1 + a - m - v,$$

where positivity requires

$$(2.5.23) \qquad \max\{0, m + v - 1\} \le a \le \min\{m, v\}.$$

Since μ and v are discrete the integral in equation 2.5.6 becomes a sum and we obtain

$$(2.5.24) \qquad W_\alpha\left(\mu, v\right) = \left(2^\alpha \inf_a (p_a(1, -1) + p_a(-1, 1))\right)^{\frac{1}{\alpha}}$$

$$(2.5.25) \qquad = 2\left(\inf_a (m + v - 2a)\right)^{\frac{1}{\alpha}}$$

$$(2.5.26) \qquad = 2|m - v|^{\frac{1}{\alpha}}.$$

We take the formula for the moments from ref. [22].

Definition 2.5.2 (Moments). For $n \in \mathbb{N}$ the the nth moment of a probability measure $\mu : \mathscr{B}(\mathbb{R}) \to [0, 1]$, on the reals is defined by the integral

$$(2.5.27) \qquad \mu[n] := \int_{\mathbb{R}} x^n d\mu(x).$$

In general the even moments may be real numbers or positive infinity, whereas the odd moments may be real, positive or negative infinity, or undefined, for example in the case of the Cauchy distribution. In the case where the probability measure is dominated by the familiar Lebesgue measure, that is where there exists a probability density function $p : \mathbb{R} \to [0, 1]$ such that

$$(2.5.28) \qquad \mu(X) = \int_X p(x) dx,$$

the formula for the moments becomes

$$(2.5.29) \qquad \mu[n] := \int_{\mathbb{R}} x^n p(x) dx.$$

If the first and second moments of a probability measure exist and are finite then we can define the variance

$$(2.5.30) \qquad \Delta^2 \mu := \mu[2] - \mu[1]^2,$$

which we will use extensively in chapter 3.

An application of the Wasserstein metric allows a generalisation of the variance to probability distributions with outcome sets which are not subsets of $\mathbb{R}$. To motivate this we consider the simplest case which can not be embedded in the real line; an observable whose outcome set is the set of points on the unit circle $\mathbb{T}$. The circle differs from a closed interval $[a - \pi, a + \pi]$ only by identifying the endpoints and is given the structure of a metric space by defining the quantity

$$(2.5.31) \qquad d(x_1, x_2) := \min_{n \in \{-1, 0, 1\}} |x_1 + 2n\pi - x_2|,$$

where the minimisation reflects the fact that two points may be connected by arcs either way around the circle. We show there is no way to define the variance of a probability distribution on the unit circle by considering the uniform distribution, to define the variance one first needs to define a mean, and there is no unique way to assign a mean to the uniform distribution over the circle. Nonetheless, there is a natural sense in which some distributions on $\mathbb{T}$ are more concentrated than others.

Definition 2.5.3. If μ is a probability measure on a metric space (A, d) and $\alpha > 1$, the α-deviation is

$$\Delta_\alpha(\mu) := \inf_{x_0 \in \mathsf{A}} W_\alpha(\mu, \delta_{x_0}), \tag{2.5.32}$$

where δ_{x_0} is a point measure supported at x_0.

The α-deviation appears in [17], and was applied in [13] to the case of covariant number and phase observables. Note that the only coupling between a measure and a point measure is the product measure, so the formula (2.5.6) simplifies substantially in this case

$$\Delta_\alpha(\mu) = \inf_{x_0 \in \mathsf{A}} \left(\int_{\mathsf{A}} d(x, x_0)^\alpha d\mu(x) \right)^{\frac{1}{\alpha}}. \tag{2.5.33}$$

We prove a piece of "folklore", giving connecting $\Delta_2(\mu)$, with the standard variance for the case where μ is a Borel probability measure on the reals.

Lemma 2.3. *If μ is a probability measure on the Borel sets of $\mathbb{R}$, with the standard topology, for which first and second moment exist and are finite then*

$$\Delta_2(\mu) = \Delta^2\mu, \tag{2.5.34}$$

where $\Delta^2\mu$ is the variance. Furthermore the infimum in equation (2.5.32) is achieved at the mean, and nowhere else.

Proof. We let μ be a Borel probability measure on $\mathbb{R}$ and consider the function

$$f : \mathbb{R} \to \mathbb{R} \tag{2.5.35}$$

$$f : x_0 \mapsto \int_{\mathbb{R}} d(x, x_0)^2 d\mu(x). \tag{2.5.36}$$

We can expand

$$f(x_0) = \int_{\mathbb{R}} d(x, x_0)^2 d\mu(x) \tag{2.5.37}$$

$$= \int_{\mathbb{R}} (x - x_0)^2 d\mu(x) \tag{2.5.38}$$

$$= \int_{\mathbb{R}} (x^2 - 2xx_0 + x_0^2) d\mu(x), \tag{2.5.39}$$

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since the first and second moment exist and are assumed to be finite we can apply the linearity of the expected value to obtain

$$(2.5.40) \qquad f(x_0) = \int_{\mathbb{R}} x^2 d\mu(x) - 2x_0 \int_{\mathbb{R}} x d\mu(x) + x_0^2 \int_{\mathbb{R}} d\mu(x)$$

$$(2.5.41) \qquad = \int_{\mathbb{R}} x^2 d\mu(x) - 2x_0 \int_{\mathbb{R}} x d\mu(x) + x_0^2.$$

This is simply a quadratic in x_0 so we can obtain the minimum and unique minimzer

$$(2.5.42) \qquad \inf_{x_0} f(x_0) = f\left(\int_{\mathbb{R}} x d\mu(x)\right)$$

$$(2.5.43) \qquad = \int_{\mathbb{R}} x^2 d\mu(x) - \left(\int_{\mathbb{R}} x d\mu(x)\right)^2,$$

which are just the variance and mean, respectively. ∎

Although this proof is rather trivial, and almost certainly is known else where, we have not been able to find a reference for it. In addition we emphasise it to contrast with the case of $\Delta_1(\mu)$ where the minimisation does *not* uniquely pick out the relevant central tendency, which is the median. An incorrect claim to the contrary was made in ref. [17]. A counterexample is given by the two outcome probability distribution defined by

$$(2.5.44) \qquad p(0) = p(1) = \frac{1}{2},$$

then

$$(2.5.45) \qquad \Delta_1(p) = \inf_{x_0} f(x_0),$$

where

$$(2.5.46) \qquad f(x_0) = \begin{cases} x_0 - \frac{1}{2}, & x_0 \leq 0 \\ \frac{1}{2}, & x_0 \in [0,1] \\ x_0 - \frac{1}{2}, & x_0 \geq 0. \end{cases}$$

Hence any $x_0 \in [0,1]$ is a minimizer for $f(x_0)$. The Wasserstein metric was used in the context of quantum uncertainty by Busch, Lahti and Werner in [16], with a focus on the case of canonically covariant observables $\mathbf{E}^Q$ and $\mathbf{E}^P$, and restricted to $\alpha = 2$. In [17] the same authors generalised this approach to consider arbitrary α. In these papers the authors considered both the supremum of the Wasserstein metric over all states, called the metric error, and a quantity called the calibration error. For observables for which there are states which make the induced probability distributions deterministic the calibration error is given by the maximum over those states. In general an observable may not induce a deterministic probability distribution in any state, so the calibration error is given by a limiting procedure

$$(2.5.47) \qquad \Delta_\alpha^\varepsilon(F,E) := \sup_{\rho,x} \left\{ W_\alpha\left(F^\rho, \delta_x\right) \mid W_\alpha\left(E^\rho, \delta_x\right) \right\}$$

$$(2.5.48) \qquad \Delta_\alpha^c(F,E) := \lim_{\varepsilon \to 0} \Delta_\alpha^\varepsilon(F,E)$$

The overall width is a natural measure of the broadness of a probability measure on the reals. Given $\varepsilon \in (0,1)$ we define

$$(2.5.49) \qquad W_\varepsilon(\mu) := \inf_{a,b \in \mathbb{R}} \left\{ |a-b| \, \big| \, \mu([a,b]) \geq 1-\varepsilon \right\},$$

the set bounded below by zero, and non-empty since for any ε there is an n large enough such that $\mu([-n,n]) \geq 1-\varepsilon$ so this quantity is a real number. The overall width has been studied in the context of timelimited and bandlimited functions in [50], in the quantum mechanical literature by Uffink [82], Busch et. al. [5] and Miyadera [60].

Entropic quantities have also been used to study quantum uncertainty, although the set of quantities which are called "entropies" is large, for our purposes it suffices to consider the Rényi α-entropies [68]. For a probability distribution on a finite set, these are given by

$$(2.5.50) \qquad H_\alpha(P) = \frac{1}{1-\alpha} \log \sum_i P(i)^\alpha.$$

The Rényi entropies are *Schur concave* as functions of the probability distribution. We write $P \prec Q$ if P may be written as a convex combination of permutations of Q, and say Q majorizes P in this case. Schur concavity is the property that

$$(2.5.51) \qquad P \prec Q \implies H_\alpha(P) \geq H_\alpha(Q),$$

roughly speaking the entropy will be larger for a more "spread out" distribution than a more concentrated one.

Given a distance measure δ on probability distributions one can define a distance measure on quantum observables by choosing a relevant set of states $S \subseteq \mathscr{S}(\mathscr{H})$ and setting

$$(2.5.52) \qquad \delta_S(E,F) := \sup_{\rho \in S} \delta(E^\rho, F^\rho),$$

of course the choice of the set S is highly significant and the appropriate choice will depend on the application. In general choosing a larger S makes the test more stringent. To make a classical analogy one would be unconvinced by a clock sold as being able to tell one time (per day) highly accurately, but a clock sold as being able to tell *all* times with error less than some bound is more convincing. Indeed this analogy can be made quite precise, given any two observables E and F one can perfectly reproduce the statistics E^ρ, and F^ρ in a fixed state ρ with the (trivial) observable

$$(2.5.53) \qquad J : (A,B) \mapsto E^\rho(A)F^\rho(B)I.$$

In chapter 5 the set S will be the whole state-space, and the distance measure on probability distributions will be the α-deviation given in (2.5.32). In general the choice of distance on the probability measures is also application dependent, but we note that if δ is a metric on the space of probability distributions, and S spans $\mathscr{S}\mathscr{H}$ then δ_S is a metric on the observables. Measuring differences between observables in terms of the outcome statistics was proposed by Ludwig [54], although the formulation of measurement uncertainty we are interested in in this thesis was introduced by Busch, Lahti and Werner [17].

Part I

Preparation uncertainty

Low dimensional Preparation uncertainty

3.1 Introduction

The textbook expression of the uncertainty principle is given by the standard uncertainty relation,

$$(3.1.1) \qquad \Delta A \, \Delta B \geq \frac{1}{2} \big| \langle AB - BA \rangle \big|.$$

Here A, B are self-adjoint operators representing two observables whose standard deviations ΔA, ΔB are constrained by the (modulus of the) expectation value of the commutator of A, B. This relation was originally conceived for position and momentum by Heisenberg [41], with formal proofs provided by Kennard [49] and Weyl [91]. The above general form is due to Robertson [70]; it was soon strengthened by Schrödinger [74, 73], who deduced a tighter bound by including the so-called covariance term,

$$(3.1.2) \qquad \Delta^2 A \, \Delta^2 B \geq \frac{1}{4} \big| \langle AB - BA \rangle \big|^2 + \frac{1}{4} \big(\langle AB + BA \rangle - 2 \langle A \rangle \langle B \rangle \big)^2.$$

These inequalities were originally presented for vector states from the system's Hilbert space, but also hold for mixed states, represented by density operators ρ. We use the standard notation $\langle A \rangle = \langle A \rangle_\rho = \mathrm{tr}[\rho A]$ for expectation values and $\Delta^2 A = \Delta_\rho^2 A = \langle A^2 \rangle_\rho - \langle A \rangle_\rho^2$ for variances.

For many decades, the task of providing a quantitative statement of the uncertainty principles was considered to be settled by stating the above inequalities. Still, a closer look shows that these relations do not have all the features one might justifiably require of an uncertainty bound. For instance, in the case of observables with discrete bounded spectra, both (3.1.1) and (3.1.2) reduce to trivialities: if ρ is an eigenstate of (say) A, so that $\Delta_\rho A = 0$, the inequalities entail no constraint on the value of $\Delta_\rho B$. A remedy to this particular deficiency came with

the discovery of other forms of uncertainty relations, based on the minimisation of functionals of $\Delta A, \Delta B$ other than the product [46, 56]. Another issue lies in the fact that the uncertainty of a quantity may not always be best described by the variance, or, more generally, the moments of its distribution; accordingly, new forms of uncertainty relations have been proven for alternative measures of uncertainty, such as entropies [9, 29, 55] or overall width [83]. We will illustrate another curiosity below: the limiting case of equality in (3.1.1) may not always indicate minimum uncertainty.

Rather than asking for bounds on some particular choice of uncertainty functional, such as the product or sum of uncertainties, it is of interest to know the *uncertainty region of* A *and* B, defined as the whole range of possible value pairs $(\Delta_\rho A, \Delta_\rho B)$. This notion does not seem to have considered until recently when similar problems were envisaged with respect to measurement uncertainty [11, 27, 52, 98]: the concept of *error region* was introduced as the set of *admissible* pairs of approximation errors for joint measurements of non-commuting quantities [12]. Arguably, the content of the uncertainty principle can be captured as a statement concerning the 'lower boundary' of the preparation and measurement uncertainty regions: if A, B do not commute, these regions cannot, in general, contain all points near the origin of the relevant uncertainty diagrams.

An extensive study of uncertainty regions for spin components was undertaken by Dammeier et al. [27] However, the features uncovered in these cases are not representative, as illustrated by the example we examine in section 3.4. In particular we note that if the point $(\Delta A, \Delta B) = (0, 0)$ is in the uncertainty region, then the monotone-closure procedure, taking the set of points $\{(x, y) | \exists \rho$ s.t. $x \geq \Delta_\rho A, y \geq \Delta_\rho B\}$, employed to great effect in the spin case, has the undesirable property that the closure defined is the *entire* positive quadrant.

A state dependent bound for the joint expectation values of an n-tuple of sharp, ± 1-valued observables was given by Kaniewski, Tomamichel and Wehner [47]. Since a binary probability distribution is entirely characterised by the expectation value this provides an implicit characterisation of the uncertainty region. A complete characterisation of the uncertainty region in terms of variances for pairs of observables on qubits was given by Li and Qiao [52]. However, their relation is an implicit rather than explicit one, with the expectation values and variances of each observable appearing on both sides of the inequality. Abbott et al [1] then derived the full qubit uncertainty region in a way which more readily generalises to provide (not necessarily tight) bounds in higher dimensional systems and for more than two observables.

Some analytical, as well as some semianalytical bounds on uncertainty regions were recently given by Szymański and Życzkowski [81], who also give a method for writing a saturated, state independent bound for a general "sum of variances" uncertainty relation as a polynomial root finding problem.

Here we review the case of qubit observables, providing yet another proof of a geometric flavor that immediately focuses on and highlights the extremality property that defines the

boundary of the uncertainty region (Section 3.3). We also investigate to what extent the standard uncertainty relations may or may not characterise the uncertainty region and find that the Schrödinger inequality cannot, in general, be cast in a state-independent form as defined here. The examples of pairs of qutrit observables given in Section 3.4 show that structural features found in the qubit case are no longer present in higher dimensions, for example the uncertainty region for two sharp, ± 1-valued qubit observables contains the origin if and only if they commute.

The purpose of the present work is to give an accessible introduction of the subject of uncertainty regions, offering worked examples for pairs of observables in low-dimensional Hilbert spaces. We also explore the logical relation between characterisations of uncertainty regions and standard uncertainty relations.

The section is organised as follows. After a brief review of the uncertainty region for the position and momentum of a particle on the line (Section 3.2.1), we give a general definition of the uncertainty region (Section 3.2.2) and proceed to consider the qubit case in some detail (Section 3.3). We then proceed to determine uncertainty regions for some pairs of qutrit observables, noting interesting contrasts with the case of qubit observables (Section 3.4). We conclude with a summary and some general observations (Section 3.5).

3.2 Uncertainty regions

3.2.1 Warm-up: a review of position and momentum

The Heisenberg uncertainty relation for position $\mathbf{Q}$ and momentum $\mathbf{P}$ of a particle on a line is given by the inequality (3.1.1),

$$(3.2.1) \qquad\qquad \Delta_\rho \mathbf{Q} \Delta_\rho \mathbf{P} \geq \frac{\hbar}{2},$$

valid for all states ρ for which both variances are finite. This relation is tight in the following sense: for any pair of numbers $(\Delta\mathbf{Q}, \Delta\mathbf{P})$ with $\Delta\mathbf{Q}\Delta\mathbf{P} \geq \hbar/2$, there exists a state ρ such that $\Delta\mathbf{Q} = \Delta_\rho\mathbf{Q}$ and $\Delta\mathbf{P} = \Delta_\rho\mathbf{P}$. In particular, points of the lower bounding hyperbola branch in the positive quadrant of the $\Delta\mathbf{Q}$-$\Delta\mathbf{P}$-plane are realized by pure states, $\rho = |\psi\rangle\langle\psi|$, where the unit vector ψ represents a Gaussian wave function. Moreover, it is not hard to show that every point in the area above the hyperbola can be realized by some quantum state, so that the whole uncertainty region for position and momentum is described by the uncertainty relation (3.2.1) (Fig. 3.1).

It is interesting to note that the inequality (3.2.1) can be equivalently recast in the form of *additive* uncertainty relations (Paul Busch, personal communication).

Theorem 3.1. *Let $\ell > 0$ be an arbitrary fixed parameter with the dimension of length, then*

$$(3.2.2) \qquad \frac{\Delta_\rho \mathbf{Q}}{\ell} + \frac{\ell \Delta_\rho \mathbf{P}}{\hbar} \geq \sqrt{2},$$

$$(3.2.3) \qquad \frac{\Delta_\rho^2 \mathbf{Q}}{\ell^2} + \frac{\ell^2 \Delta_\rho^2 \mathbf{P}}{\hbar^2} \geq 1.$$

Proof. The proof of this equivalence follows from an elementary algebraic observation: given arbitrary $\xi, \eta > 0$ we have the simple identity

$$(3.2.4) \qquad \frac{\xi}{x} + x\eta = \left(\sqrt{\frac{\xi}{x}} - \sqrt{x\eta} \right)^2 + 2\sqrt{\xi\eta},$$

valid for all $x > 0$. This quantity assumes its minimal value $2\sqrt{\xi\eta}$ at $x = \sqrt{\xi/\eta}$. Therefore, if C is a positive constant, then

$$(3.2.5) \qquad \xi\eta \geq C \quad \Longleftrightarrow \quad \forall x > 0 : \frac{\xi}{x} + x\eta \geq 2\sqrt{C}.$$

Putting $(\xi, \eta, C) = (\Delta^2 \mathbf{Q}/\ell^2, \ell^2 \Delta^2 \mathbf{P}/\hbar^2, 1/2)$ or $= (\Delta^2 \mathbf{Q}/\ell^2, \ell^2 \Delta^2 \mathbf{P}/\hbar^2, 1/4)$ and choosing $x = 1$, we see that the uncertainty relation (3.2.1) entails (3.2.2) and (3.2.3), for every state ρ via the equivalence (3.2.5).

To obtain the reverse implication, we have to make the stronger assumption that one of the additive inequalities, say (3.2.2), holds *for all ρ*, for some fixed value ℓ. To show that then this inequality holds for all ℓ, we replace ℓ with $\ell' \equiv x\ell$, with $x > 0$. Using the unitary scaling transformation,

$$(3.2.6) \qquad U_\tau = \exp\left[\frac{i}{2\hbar} \tau(\mathbf{Q}\mathbf{P} + \mathbf{P}\mathbf{Q}) \right], \quad \tau = \ln x,$$

we have $U_\tau^* \mathbf{Q} U_\tau = \mathbf{Q}/x \equiv \mathbf{Q}_x$, $U_\tau^* \mathbf{P} U_\tau = x\mathbf{P} \equiv \mathbf{P}_x$, and set $\rho_x = U_\tau \rho U_\tau^*$. We then calculate:

$$(3.2.7) \qquad \frac{\Delta_\rho \mathbf{Q}}{x\ell} + \frac{x\ell \Delta_\rho \mathbf{P}}{\hbar} = \frac{\Delta_\rho \mathbf{Q}_x}{\ell} + \frac{\ell \Delta_\rho \mathbf{P}_x}{\hbar} = \frac{\Delta_{\rho_x} \mathbf{Q}}{\ell} + \frac{\ell \Delta_{\rho_x} \mathbf{P}}{\hbar} \geq \sqrt{2}.$$

Therefore, using (3.2.5), we conclude that (3.2.1) follows from (3.2.2) (and similarly from (3.2.3)). ∎

Geometrically, the limiting case of equality in (3.2.2) represents a family of straight lines tangent to the hyperbola plotted in a $\Delta \mathbf{Q} - \Delta \mathbf{P}$-diagram given by $\Delta \mathbf{Q} \Delta \mathbf{P} = \hbar/2$; the totality of these tangents defines the hyperbola. Similarly, the second additive inequality bound (3.2.3) gives a family of ellipses (with axes given by the coordinate axes) tangent to the hyperbola, again defining it (see Fig. 3.1). We conclude that Heisenberg's uncertainty relation or any of its additive equivalents completely determine the position-momentum uncertainty region.
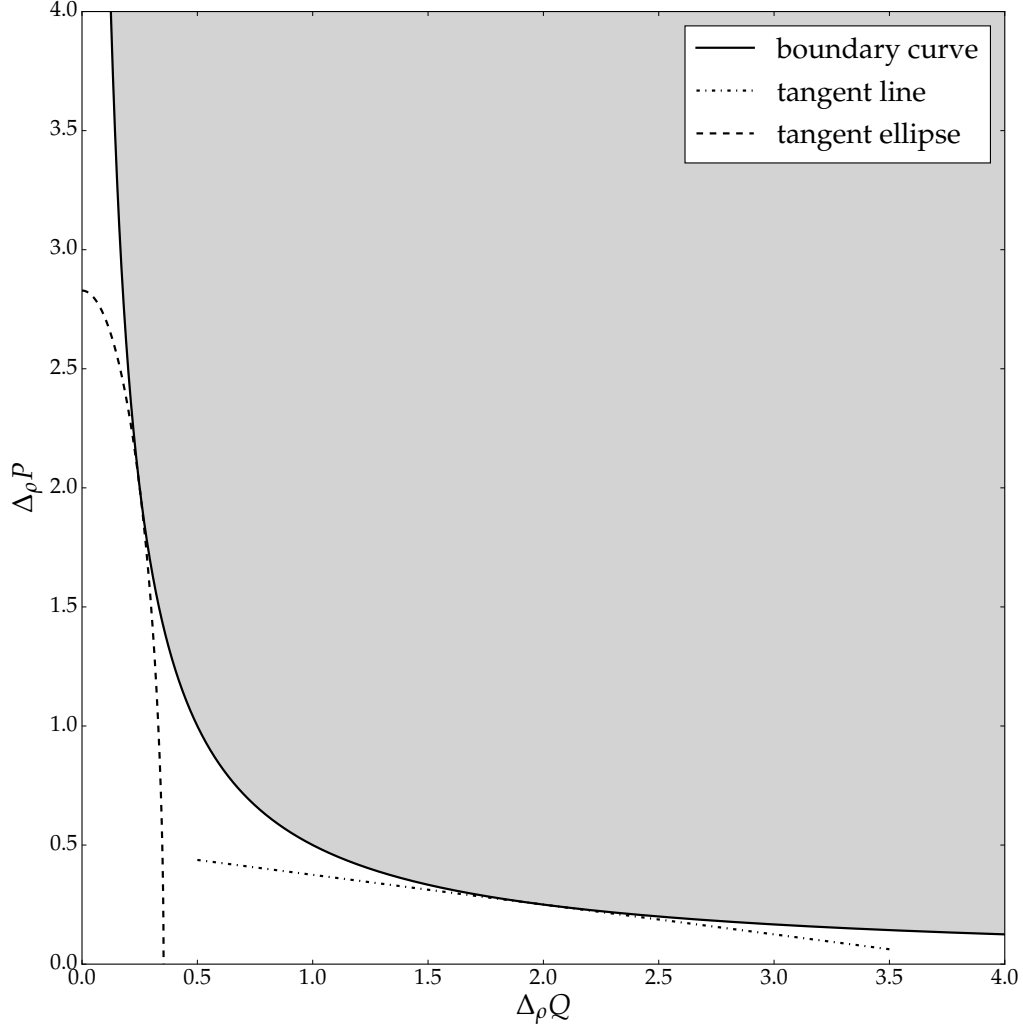
Figure 3.1: The uncertainty region for the standard deviations of position and momentum (in units where $\hbar = 1$). The solid boundary line represents the hyperbola $\Delta \mathbf{Q} \Delta \mathbf{P} = \frac{1}{2}$, and the dash-dotted and dotted curves show examples of the tangential straight and elliptic line segments represented by the bounds given in (3.2.2) and (3.2.3), respectively.

3.2.2 Uncertainty region: general definition

We seek to explore further the feature of tightness of an uncertainty relation and so adopt the following definitions (see, e.g., Ref. [1]). We will understand tightness in the sense that the given uncertainty relation fully characterises the set of admissible uncertainty pairs. In order for an inequality for the uncertainties to achieve this, it is necessary that the only state-dependent terms are the uncertainties themselves; hence such inequalities are of the form

$f(\Delta A, \Delta B, A, B) \geq 0$. As the reference to ρ can then be dropped, we refer to such uncertainty relations as *state-independent*, in line with the terminology introduced in Ref. [1]. The term *tight* is sometimes used to describe an inequality for a set of variables where the limiting case of equality can be reached for some values; here instead we refer to this situation as *saturation* of the inequality.

Definition 3.1. The *(preparation) uncertainty region* for a pair of observables **A** and **B** is the set of points $(\Delta A, \Delta B) \in \mathbb{R}^2$ that can be realised by some quantum state, $\rho \in \mathscr{S}(\mathscr{H})$, that is,

$$(3.2.8) \qquad \mathrm{PUR}_\Delta(A, B) = \left\{ (\Delta A, \Delta B) \,|\, \exists \rho \in \mathscr{S}(\mathscr{H}) : \Delta A = \Delta_\rho A, \ \Delta B = \Delta_\rho B \right\}.$$

Definition 3.2. A state-independent uncertainty relation, given by an equality, inequality or set of such, for the uncertainties $\Delta_\rho A$, $\Delta_\rho B$ of observables **A**, **B** will be called *tight* if it is satisfied for exactly the points $(\Delta A, \Delta B)$ inside the uncertainty region.

Although we focus here mostly on pairs of observables the definitions may be generalised to n observables in the obvious way. Furthermore, one may also take alternative measures of uncertainty instead of the standard deviations. We will occasionally use the variance instead of the standard deviation, where the former is more appropriate.

It is natural to ask whether the tightness of the inequality (3.1.1) (and hence (3.1.2)) extends beyond the case of position and momentum. More generally, one can ask for any pair (or family) of observables whether the associated uncertainty region can be characterised by suitable uncertainty relations (which then would be tight).

For the purposes of finding expressions of the uncertainty principle, it is sufficient to focus on specifying the curve defined by fixing the value of ΔA and finding $\rho \in \mathscr{S}(\Delta A) := \{\rho \,|\, \Delta_\rho A = \Delta A\}$ such that $\Delta_\rho B$ is minimized:

$$(3.2.9) \qquad \Delta B_{\min} \equiv \min \left\{ \Delta_\rho B \,|\, \rho \in \mathscr{S}(\Delta A) \right\}.$$

Assuming (as we do henceforth) that the underlying Hilbert space is finite-dimensional, the set of states $\mathscr{S}(\mathscr{H})$ is compact in any norm topology (trace norm, operator norm, etc.). Therefore, the continuity of the map $\rho \mapsto (\Delta_\rho A, \Delta_\rho B)$ ensures that the preparation uncertainty region and the subset of states $\mathscr{S}(\Delta A)$ are compact. It follows that the minimum in (3.2.9) exists. Hence the uncertainty region has a well-defined lower boundary curve (and similarly upper and side boundary curves).

We illustrate cases where there are non-trivial *upper* bounds for $\Delta_\rho B$ for some values of $\Delta_\rho A$. Additionally, when examining qutrit observables in section 3.4, we discover that the uncertainty region is not necessarily of a 'simple' shape, such as a convex set. In these cases the uncertainty region is too complicated to be conveniently described by a single inequality, but may be given, for example, in terms of its bounding curves.

3.3 Optimal qubit uncertainty relations

We consider sharp qubit observables with outcomes (eigenvalues) ± 1. These are represented as Hermitian operators (or 2×2-matrices) of the form $A = \boldsymbol{a} \cdot \boldsymbol{\sigma} = a_x \sigma_x + a_y \sigma_y + a_z \sigma_z$, where vector $\boldsymbol{a}$ has Euclidean length $\|\boldsymbol{a}\| = 1$ and $\sigma_x, \sigma_y, \sigma_z$ denote the Pauli matrices on $\mathbb{C}^2$. A general qubit state may be expressed as the density operator

$$(3.3.1) \qquad \rho = \frac{1}{2}(I + \boldsymbol{r} \cdot \boldsymbol{\sigma}), \quad \|\boldsymbol{r}\| = r \le 1,$$

where I denotes the identity operator (unit matrix). Note that ρ is a pure state if and only if $\|\boldsymbol{r}\| = 1$.

For $A = \boldsymbol{a} \cdot \boldsymbol{\sigma}$, we have $\langle A \rangle_\rho = \boldsymbol{a} \cdot \boldsymbol{r}$ and, since $A^2 = I$,

$$(3.3.2) \qquad \Delta_\rho^2 A = 1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2 = 1 - \|\boldsymbol{r}\|^2 + \|\boldsymbol{r} \times \boldsymbol{a}\|^2.$$

We recall that for unit 3-vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ separated by angle θ we have $\boldsymbol{a} \cdot \boldsymbol{b} = \cos\theta$ and $\|\boldsymbol{a} \times \boldsymbol{b}\| = \sin\theta$. We also note the operator norm of the commutator of A, B is given by

$$(3.3.3) \qquad \big\|[A, B]\big\| = 2\|\boldsymbol{a} \times \boldsymbol{b}\|,$$

which suggests that $\|\boldsymbol{a} \times \boldsymbol{b}\|$, area of the parallelogram spanned by $\boldsymbol{a}$ and $\boldsymbol{b}$, is the relevant quantity to measure the degree of noncommutativity (incompatibility) of A and B. It is interesting to note that uncertainty relations have been derived for n observables obtained from the position and momentum of the particle on a line where the lower bound is given by the volume of an n dimensional parallelepiped [48].

3.3.1 Uncertainty bounds for $\sigma_x, \sigma_y, \sigma_z$

Considering the variances of $\sigma_x, \sigma_y, \sigma_z$ in a general state ρ,

$$(3.3.4) \qquad \Delta_\rho^2 \sigma_x = 1 - r_x^2, \quad \Delta_\rho^2 \sigma_y = 1 - r_y^2, \quad \Delta_\rho^2 \sigma_z = 1 - r_z^2,$$

it is easy to see that the positivity condition for ρ, $r_x^2 + r_y^2 + r_z^2 \le 1$, is in fact equivalent to the following additive uncertainty relation:

$$(3.3.5) \qquad \Delta_\rho^2 \sigma_x + \Delta_\rho^2 \sigma_y + \Delta_\rho^2 \sigma_z = 3 - \|\boldsymbol{r}\|^2 \ge 2.$$

This inequality is saturated if and only if ρ is a pure state ($r^2 = 1$). Given that the standard deviations $\Delta_\rho \sigma_k \in [0, 1]$, the uncertainty region for the triple $(\sigma_x, \sigma_y, \sigma_z)$ is given as the complement of the open ball at the origin with radius $\sqrt{2}$ intersected with the unit cube $[0, 1] \times [0, 1] \times [0, 1]$ (Fig. 3.2). The inequality (3.3.5) is an instance of a general triple uncertainty relation for the components of a spin-s system, with the bound for the sum of variances being s, as shown in Ref. [42].
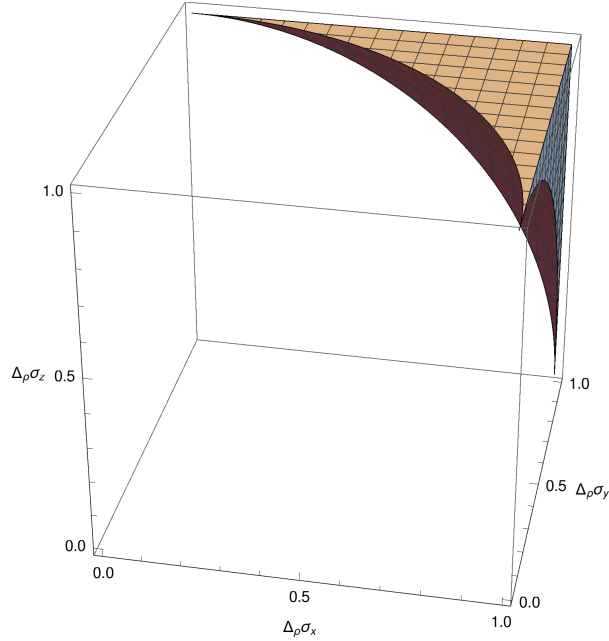
Figure 3.2: The uncertainty region for the standard deviations of the qubit triple $(\sigma_x, \sigma_y, \sigma_z)$. Note that the top surface with $\Delta\sigma_z = 1$, shows the uncertainty region for the pair σ_x, σ_y, determined by $\Delta_\rho^2\sigma_x + \Delta_\rho^2\sigma_y \geq 1$, which can be filled with states whose Bloch vectors have component $r_z = 0$.

We briefly revisit and compare the Heisenberg and Schrödinger inequalities for spin components. The uncertainty relation (3.1.1) for σ_x, σ_y is equivalent to

$$(3.3.6) \qquad \Delta_\rho^2\sigma_x \Delta_\rho^2\sigma_y \geq |\langle\sigma_z\rangle_\rho|^2 = 1 - \Delta_\rho^2\sigma_z.$$

We note that the lower bound on the right hand side becomes zero if $r_z = 0$, in which case this inequality gives no constraint on the variances on the left hand side. However, using (3.3.5), we obtain

$$(3.3.7) \qquad \Delta_\rho^2\sigma_x \Delta_\rho^2\sigma_y \geq \Delta_\rho^2\sigma_x\big(2 - \Delta_\rho^2\sigma_x - \Delta_\rho^2\sigma_z\big) \geq \Delta_\rho^2\sigma_x\big(1 - \Delta_\rho^2\sigma_x\big).$$

We see that the bound is now nontrivial for all ρ with $\Delta_\rho\sigma_x = \Delta\sigma_x \in (0,1)$. It can be as large as $1/4$, which is obtained when $\boldsymbol{r} = (\pm 1, \pm 1, 0)/\sqrt{2}$. The above inequality is equivalent to the following, which is also entailed directly by (3.3.5) bearing in mind that $\Delta_\rho^2\sigma_z \leq 1$:

$$(3.3.8) \qquad \Delta_\rho^2\sigma_x + \Delta_\rho^2\sigma_y \geq 1.$$

From this, we can straightforwardly obtain the minimum (3.2.9) for $\Delta_\rho^2\sigma_y$ given a fixed $\Delta_\rho^2\sigma_x \in (0,1)$. In fact, $\Delta_\rho^2\sigma_y$ is minimized when $\Delta_\rho^2\sigma_y = 1 - \Delta_\rho^2\sigma_x$. This is equivalent to $r_x^2 + r_y^2 = 1$, which entails $r_z = 0$, that is, $\Delta_\rho^2\sigma_z = 1$. This means, in particular, that the bound given by (3.3.6) becomes trivial and that given by (3.1.2) is tight.

It is instructive to consider the conditions under which the Heisenberg inequality (3.3.6) is saturated. This gives $(1 - r_x^2)(1 - r_y^2) = r_z^2$, or $1 + r_x^2 r_y^2 = r_x^2 + r_y^2 + r_z^2$. Since the right-hand side is never greater than 1 and the left hand side never less than 1, both sides must be equal to 1 and, therefore either $r_x = 0$ or $r_y = 0$. If r_x is fixed and non-zero, then $r_y = 0$, which is to say that $\Delta_\rho^2 \sigma_y = 1$.

Note that here $\Delta_\rho^2 \sigma_y$ is maximal rather than minimal. Saturation of the standard uncertainty relation for these observables thus leads to maximising the uncertainty product instead of minimising it, as one might, naively, have expected. In contrast, equality in (3.3.8) forces minimality of the uncertainty product. We also see that (3.3.6) forces maximality $\Delta_\rho^2 \sigma_x = \Delta_\rho^2 \sigma_y = 1$ by requiring minimal uncertainty for σ_z, whereas (3.3.8) does not stipulate this.

Taking into account the natural upper bound of 1 for the variances, the inequality (3.3.8) is tight, that is, it captures exactly the uncertainty region for σ_x, σ_y, while (3.3.6) does not. (As we observed above, (3.3.6) does not set a positive lower bound for $\Delta_\rho^2 \sigma_y$ when $\Delta_\rho^2 \sigma_z = 1$.)

Since $0 \le \left(1 - \Delta_\rho^2 \sigma_x\right)\left(1 - \Delta_\rho^2 \sigma_y\right)$, we have

$$(3.3.9) \qquad \Delta_\rho^2 \sigma_x \Delta_\rho^2 \sigma_y \ge \Delta_\rho^2 \sigma_x + \Delta_\rho^2 \sigma_y - 1 \ge 1 - \Delta_\rho^2 \sigma_z,$$

where the latter inequality is obtained from $\|\boldsymbol{r}\|^2 \le 1$ or the equivalent relation (3.3.5). It follows that, just like (3.3.8), (3.3.6) is also a consequence of (and indeed weaker than) (3.3.5).

The fact that (3.3.5) implies (3.3.6) should not be surprising once one realises that the former inequality is indeed equivalent to the Schrödinger relation (3.1.2), which takes the following form in the present case

$$(3.3.10) \qquad \Delta_\rho^2 \sigma_x \Delta_\rho^2 \sigma_y \ge \langle \sigma_z \rangle_\rho^2 + \langle \sigma_x \rangle_\rho^2 \langle \sigma_y \rangle_\rho^2 = \left(1 - \Delta_\rho^2 \sigma_z\right) + \left(1 - \Delta_\rho^2 \sigma_x\right)\left(1 - \Delta_\rho^2 \sigma_y\right).$$

This is equivalent to

$$(3.3.11) \qquad \Delta_\rho^2 \sigma_x \Delta_\rho^2 \sigma_y \ge 2 - \left(\Delta_\rho^2 \sigma_x + \Delta_\rho^2 \sigma_y + \Delta_\rho^2 \sigma_z\right) + \Delta_\rho^2 \sigma_x \Delta_\rho^2 \sigma_y,$$

and hence to (3.3.5), and ultimately to $\|\boldsymbol{r}\|^2 \le 1$, anticipating the results of section 3.3.3. We summarise in proposition 3.1

Proposition 3.1 (Summary of uncertainty bounds for orthogonal Pauli observables)**.**

1. *The Schrödinger inequality* (3.3.10) *(but not the Heisenberg inequality* (3.3.6)*) for* σ_x, σ_y *determines their uncertainty region.*

2. *Saturation of the Heisenberg inequality does not entail minimal, but instead maximal, uncertainty (i.e., maximal* $\Delta \sigma_y$ *given* $\Delta \sigma_x \notin \{0, 1\}$*).*

3. *The uncertainty region for* σ_x, σ_y *is the intersection of the unit square* $[0,1] \times [0,1]$ *with the complement of the open unit ball* $\Delta^2 \sigma_x + \Delta^2 \sigma_y < 1$. *The lower boundary is reached exactly*

for pure states with $\Delta\sigma_z = 1$, which entails the vanishing of the commutator term in the Heisenberg inequality (3.3.8) (which therefore becomes trivial at minimum uncertainty). In this case, one has equality in the Schrödinger relation, and the uncertainty bound is found to be entirely due to the covariance term.

4. *The Schrödinger inequality, due to its equivalence with (3.3.5), also determines the triple uncertainty region for $\sigma_x, \sigma_y, \sigma_z$, Fig. 3.2.*

5. *Saturation of the Schrödinger inequality and the equivalent triple uncertainty relation (3.3.5) is given exactly on the set of pure states. Hence, all pure states are minimum uncertainty states for the sum uncertainty relation for the triple $\sigma_x, \sigma_y, \sigma_z$.*

3.3.2 Uncertainty region for pairs of ±1-valued qubit observables

We now consider general observables represented as $A = \boldsymbol{a} \cdot \boldsymbol{\sigma}$, $B = \boldsymbol{b} \cdot \boldsymbol{\sigma}$ where $\boldsymbol{a}$ and $\boldsymbol{b}$ are unit vectors but no longer assumed to be orthogonal. Observables of this form are sufficient to explore the shapes of uncertainty regions since any two outcome qubit observable may be simulated by one of this form using classical post processing (relabelling the outcomes ±1 and adding classical noise).

We begin by noting some simple known examples of state-independent uncertainty relations for the pair A, B given in Ref. [15]:

$$(3.3.12) \qquad \Delta A + \Delta B \;\geq\; \tfrac{1}{2}\big\|[A,B]\big\|,$$

$$(3.3.13) \qquad \Delta^2 A + \Delta^2 B \;\geq\; 1 - \sqrt{1 - \tfrac{1}{4}\big\|[A,B]\big\|^2}.$$

While these are easily proven by elementary means, it is equally easy to see that they are not tight; they only touch the actual lower boundary curve of the uncertainty region at isolated points. Nevertheless they are of a simple form and illustrate the concept of a state-independent uncertainty bound. In the remainder of this subsection we will derive the exact uncertainty region, given in theorem 3.2.

Theorem 3.2. *Given a pair of qubit observables $A = \boldsymbol{a} \cdot \boldsymbol{\sigma}$, $B = \boldsymbol{b} \cdot \boldsymbol{\sigma}$ as well as a fixed uncertainty $\Delta_\rho A = \Delta A$ we have*

$$(3.3.14) \quad \left|\Delta A(\boldsymbol{a} \cdot \boldsymbol{b}) - \|\boldsymbol{a} \times \boldsymbol{b}\|\sqrt{1 - \Delta^2 A}\right| \leq \Delta_\rho B \leq \begin{cases} \Delta A(\boldsymbol{a} \cdot \boldsymbol{b}) + \|\boldsymbol{a} \times \boldsymbol{b}\|\sqrt{1 - \Delta^2 A} & \text{if } \Delta A < \boldsymbol{a} \cdot \boldsymbol{b} \\ 1 & \text{otherwise} \end{cases}.$$

The resulting uncertainty region is plotted in Fig. 3.3.
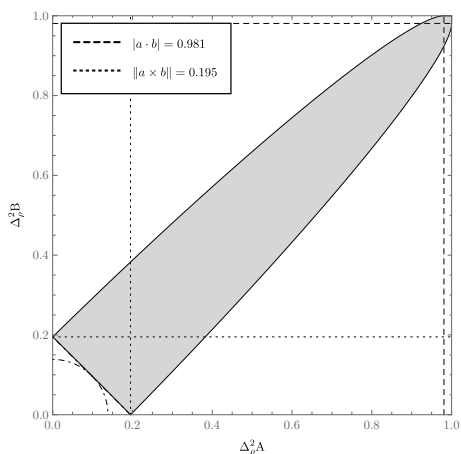
(a) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{\pi}{16}$.
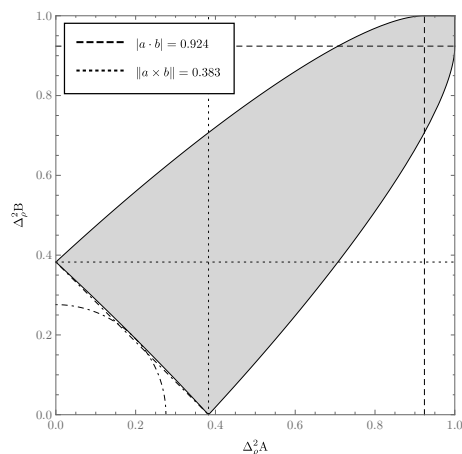
(b) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{\pi}{8}$.
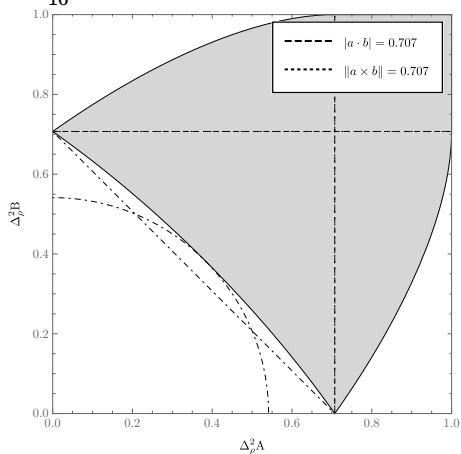
(c) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{\pi}{4}$.
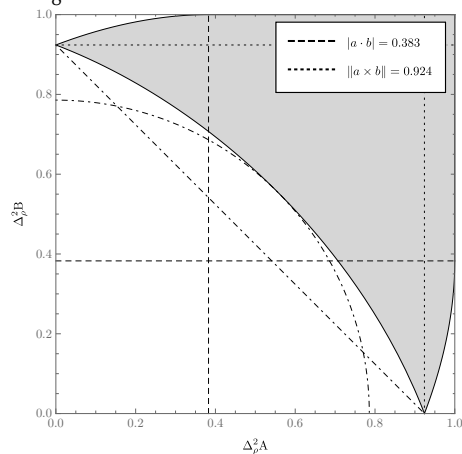
(d) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{3\pi}{8}$.
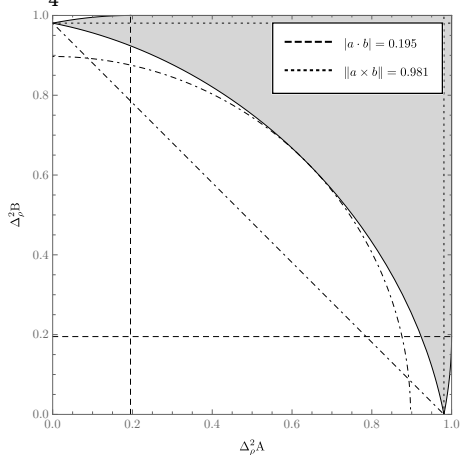
(e) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{7\pi}{16}$.
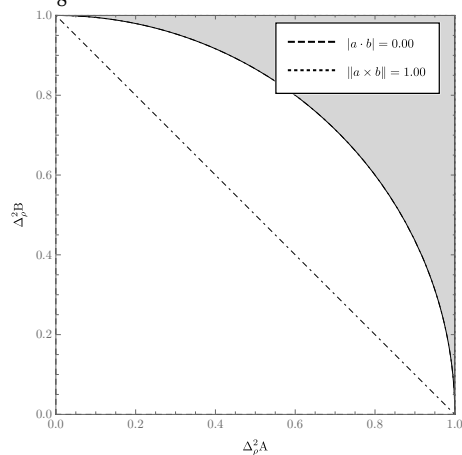
(f) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{\pi}{2}$.

Figure 3.3: Plots of the uncertainty region for sharp, ±1-valued qubit observables. The straight and curved dot-dashed lines are the previously known lower bounds (3.3.12) and (3.3.13), respectively.

In the following considerations we will make use of the identity

$$(3.3.15) \qquad \|\boldsymbol{a} \times \boldsymbol{b}\|^2 \|\boldsymbol{r}\|^2 = \big((\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{r}\big)^2 + \big\|(\boldsymbol{a} \times \boldsymbol{b}) \times \boldsymbol{r}\big\|^2,$$

which is a version of Pythagoras' law. In the special case that $\|\boldsymbol{a}\| = \|\boldsymbol{b}\| = \|\boldsymbol{r}\| = 1$ and $\boldsymbol{r} \perp \boldsymbol{a} \times \boldsymbol{b}$, this yields

$$(3.3.16) \qquad \|\boldsymbol{a} \times \boldsymbol{b}\| = \big\|\boldsymbol{b}(\boldsymbol{a} \cdot \boldsymbol{r}) - \boldsymbol{a}(\boldsymbol{b} \cdot \boldsymbol{r})\big\| = \big\|\boldsymbol{a}(\boldsymbol{a} \cdot \boldsymbol{r}) - \boldsymbol{b}(\boldsymbol{b} \cdot \boldsymbol{r})\big\|.$$

We obtain the following Lemma.

Lemma 3.1. *Let $\boldsymbol{a}, \boldsymbol{b}$ be unit vectors spanning a plane P. For any unit vector $\boldsymbol{r} \in P$, denote $\boldsymbol{a}^* = \boldsymbol{a}(\boldsymbol{a} \cdot \boldsymbol{r})$, $\boldsymbol{b}^* = \boldsymbol{b}(\boldsymbol{b} \cdot \boldsymbol{r})$ and $\boldsymbol{x} = \boldsymbol{r} - \boldsymbol{a}^*$, $\boldsymbol{y} = \boldsymbol{r} - \boldsymbol{b}^*$. Then*

$$(3.3.17) \qquad \big\|\boldsymbol{a} \times \boldsymbol{b}\big\| = \|\boldsymbol{a}^* - \boldsymbol{b}^*\| = \|\boldsymbol{x} - \boldsymbol{y}\|.$$

To describe the uncertainty region, we set out to determine the maximum and minimum values of $\Delta_\rho^2 B$ given a fixed value $\Delta^2 A$ of $\Delta_\rho^2 A$. Minimality (maximality) of $\Delta_\rho^2 B$ is equivalent to maximality (minimality) of $(\boldsymbol{r} \cdot \boldsymbol{b})^2$ whilst keeping $(\boldsymbol{r} \cdot \boldsymbol{a})^2 = 1 - \Delta^2 A$ constant. Fixing the variance of A restricts the state to be within the two disks that are the intersections of the planes $\boldsymbol{r} \cdot \boldsymbol{a} = \pm\sqrt{1 - \Delta^2 A}$ with the Bloch sphere. We may assume $\boldsymbol{a} \cdot \boldsymbol{b} \geq 0$. For the determination of minimal and maximal $\Delta_\rho B$ it will be sufficient to focus on the disks of constant ΔA with $\boldsymbol{r} \cdot \boldsymbol{a} \geq 0$, and look for the two disks of constant $\boldsymbol{r} \cdot \boldsymbol{b}$ which intersect the former disk in just one point. The resulting vectors $\boldsymbol{r}_0, \boldsymbol{r}_1$ (which are or can be chosen to lie in the plane spanned by $\boldsymbol{a}, \boldsymbol{b}$) are those giving the largest, resp. smallest, non-negative value of $\boldsymbol{b} \cdot \boldsymbol{r}$ within the disk of vectors satisfying $\boldsymbol{r} \cdot \boldsymbol{a} = \sqrt{1 - \Delta^2 A}$.

Figure 3.4 shows the Bloch vectors $\boldsymbol{r}_0, \boldsymbol{r}_1$ corresponding to the states that minimize, resp. maximize $\Delta_\rho B$. These are unit vectors in the plane spanned by $\boldsymbol{a}, \boldsymbol{b}$ (except for the cases where the maximum $\Delta_\rho B = 1$ and $\Delta A > \boldsymbol{a} \cdot \boldsymbol{b}$). There are four constellations of interest according to distinct regions of increasing values of ΔA. We determine the minimal and maximal values $\Delta B_{\min}, \Delta B_{\max}$ in each case. To be specific, we assume $\boldsymbol{a} \cdot \boldsymbol{b} \geq \|\boldsymbol{a} \times \boldsymbol{b}\|$, that is, $\theta \leq \pi/4$; the case $\theta > \pi/4$ is treated similarly. As evident from Figures 3.5 and 3.6, we have $\|\boldsymbol{x}\| = \Delta A$, and $\|\boldsymbol{y}\| = \Delta B_{\min}$, resp. $\|\boldsymbol{y}\| = \Delta B_{\max}$. Then repeated application of Eq. 3.3.17 and using the relation $\boldsymbol{x} \cdot \boldsymbol{y} = \pm \boldsymbol{a} \cdot \boldsymbol{b} \|\boldsymbol{x}\| \|\boldsymbol{y}\|$ with the appropriate choice of sign gives the following equations

(a) $\boldsymbol{a}\cdot\boldsymbol{r}>\boldsymbol{a}\cdot\boldsymbol{b} \iff \Delta\mathrm{A}<\|\boldsymbol{a}\times\boldsymbol{b}\|$

(b) $\boldsymbol{a}\cdot\boldsymbol{r}=\boldsymbol{a}\cdot\boldsymbol{b}>\boldsymbol{a}\cdot\boldsymbol{b}'=\|\boldsymbol{a}\times\boldsymbol{b}\| \iff \Delta\mathrm{A}=\|\boldsymbol{a}\times\boldsymbol{b}\|$

(c) $\boldsymbol{a}\cdot\boldsymbol{r}=\boldsymbol{a}\cdot\boldsymbol{b}'=\|\boldsymbol{a}\times\boldsymbol{b}\| \iff \Delta\mathrm{A}=\boldsymbol{a}\cdot\boldsymbol{b}$

(d) $0<\boldsymbol{a}\cdot\boldsymbol{r}<\boldsymbol{a}\cdot\boldsymbol{b}' \iff \Delta\mathrm{A}>\boldsymbol{a}\cdot\boldsymbol{b}$
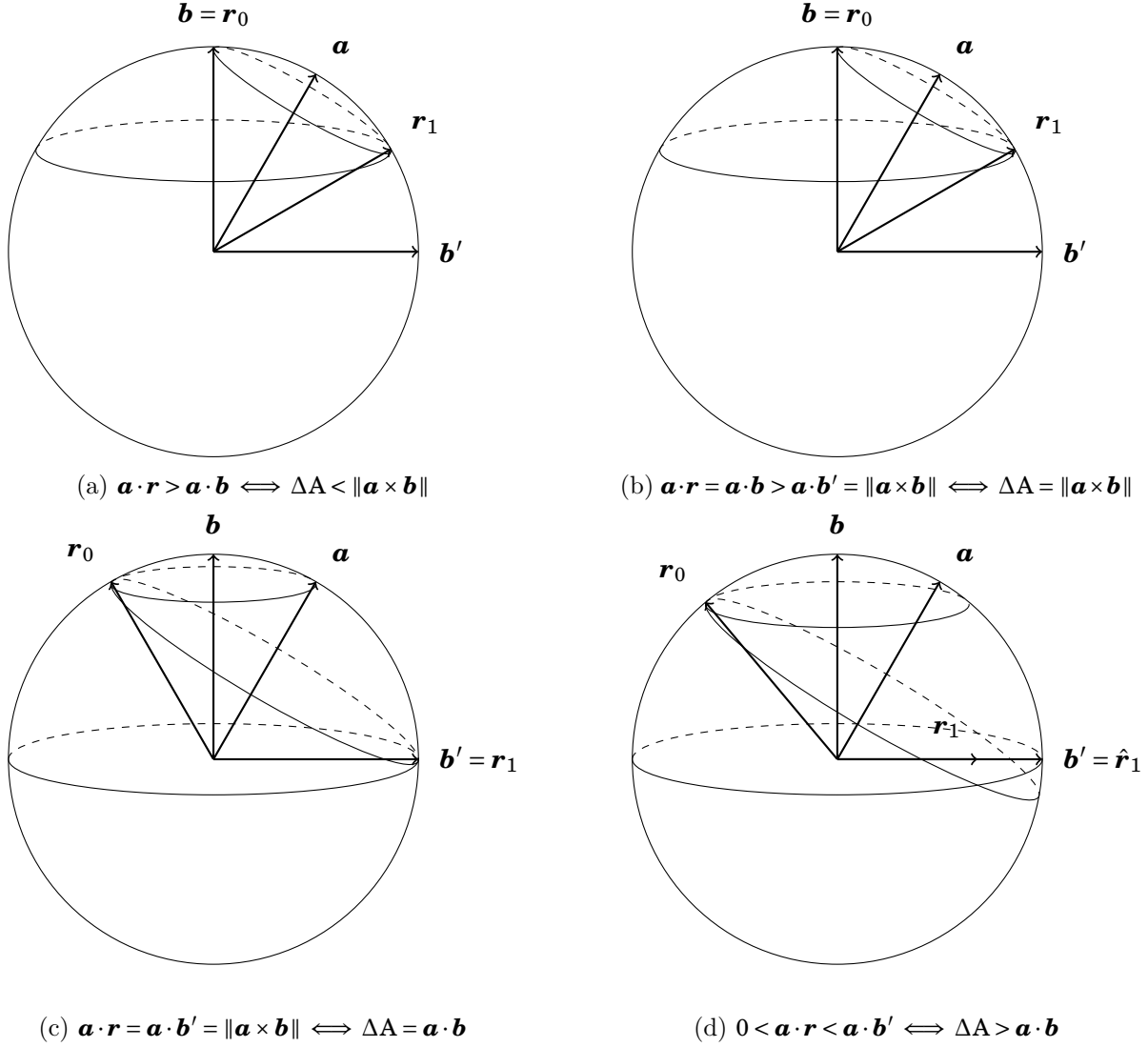
Figure 3.4: Determining the locations of Bloch vectors $\boldsymbol{r}_0,\boldsymbol{r}_1$ (in the plane spanned by $\boldsymbol{a},\boldsymbol{b}$) for states minimizing and maximizing $\Delta_\rho^2\mathrm{B}$ within the set of states with $\Delta_\rho\mathrm{A}=\Delta\mathrm{A}$. We consider the case $\boldsymbol{a}\cdot\boldsymbol{b}>\|\boldsymbol{a}\times\boldsymbol{b}\|$ only (shown here for $\theta=\frac{\pi}{6}$).

for $\Delta\mathrm{B}_{\min}$, $\Delta\mathrm{B}_{\max}$

$$(3.3.18) \qquad 0\le\Delta\mathrm{A}\le\|\boldsymbol{a}\times\boldsymbol{b}\| \iff 1\ge\boldsymbol{a}\cdot\boldsymbol{r}\ge\boldsymbol{a}\cdot\boldsymbol{b}$$

$$(3.3.19) \qquad \implies \|\boldsymbol{a}\times\boldsymbol{b}\|^2=\Delta^2\mathrm{A}+\Delta^2\mathrm{B}_{\min}+2\boldsymbol{a}\cdot\boldsymbol{b}\,\Delta\mathrm{A}\Delta\mathrm{B}_{\min}$$

$$(3.3.20) \qquad \|\boldsymbol{a}\times\boldsymbol{b}\|\le\Delta\mathrm{A}\le 1 \iff \boldsymbol{a}\cdot\boldsymbol{b}\ge\boldsymbol{a}\cdot\boldsymbol{r}\ge 0$$

$$(3.3.21) \qquad \implies \|\boldsymbol{a}\times\boldsymbol{b}\|^2=\Delta^2\mathrm{A}+\Delta^2\mathrm{B}_{\min}-2\boldsymbol{a}\cdot\boldsymbol{b}\,\Delta\mathrm{A}\Delta\mathrm{B}_{\min}$$

$$(3.3.22) \qquad 0\le\Delta\mathrm{A}\le\boldsymbol{a}\cdot\boldsymbol{b} \iff 1\ge\boldsymbol{a}\cdot\boldsymbol{r}\ge\|\boldsymbol{a}\times\boldsymbol{b}\|$$

$$(3.3.23) \qquad \implies \|\boldsymbol{a}\times\boldsymbol{b}\|^2=\Delta^2\mathrm{A}+\Delta^2\mathrm{B}_{\max}-2\boldsymbol{a}\cdot\boldsymbol{b}\,\Delta\mathrm{A}\Delta\mathrm{B}_{\max}$$

$$(3.3.24) \qquad \Delta\mathrm{A}\ge\boldsymbol{a}\cdot\boldsymbol{b} \iff \boldsymbol{a}\cdot\boldsymbol{r}\le\|\boldsymbol{a}\times\boldsymbol{b}\|$$

$$(3.3.25) \qquad \implies \Delta\mathrm{B}_{\max}=1 \quad \text{at } \boldsymbol{r}=\boldsymbol{r}_1 \text{ (in the direction of } \boldsymbol{b}'\text{).}$$
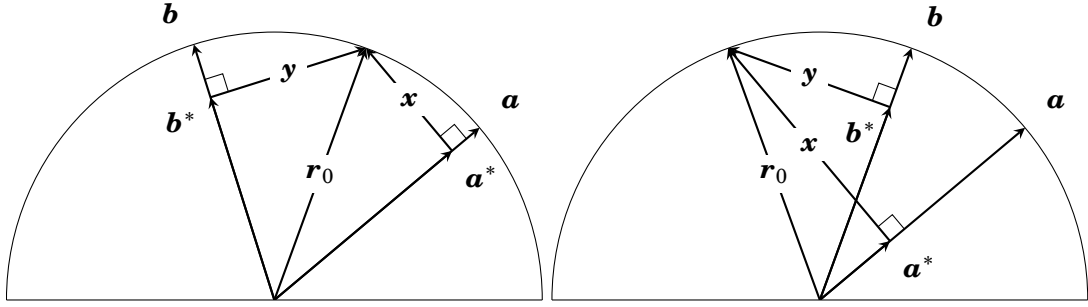
(a) Cross-section through the Bloch sphere showing the relations between the various vectors in the case where the choice of $\Delta_\rho A = \|\boldsymbol{x}\|$ fixes $\boldsymbol{r}_0$ to be between $\boldsymbol{a}$ and $\boldsymbol{b}$ to minimize $\Delta_\rho B = \|\boldsymbol{y}\|$. Note that $\boldsymbol{x} \cdot \boldsymbol{y} = -\boldsymbol{a} \cdot \boldsymbol{b} \|\boldsymbol{x}\| \|\boldsymbol{y}\|$.

(b) Cross-section through the Bloch sphere showing the relations between the various vectors in the case where the choice of $\Delta_\rho A$ fixes $\boldsymbol{r}_0$ to be outside $\boldsymbol{a}$ and $\boldsymbol{b}$ to minimize $\Delta_\rho B$. Note that $\boldsymbol{x} \cdot \boldsymbol{y} = \boldsymbol{a} \cdot \boldsymbol{b} \|\boldsymbol{x}\| \|\boldsymbol{y}\|$.

Figure 3.5: Illustration of the $\boldsymbol{r}_0$ vectors which minimize $\Delta_\rho B$ given a fixed value of $\Delta_\rho A$
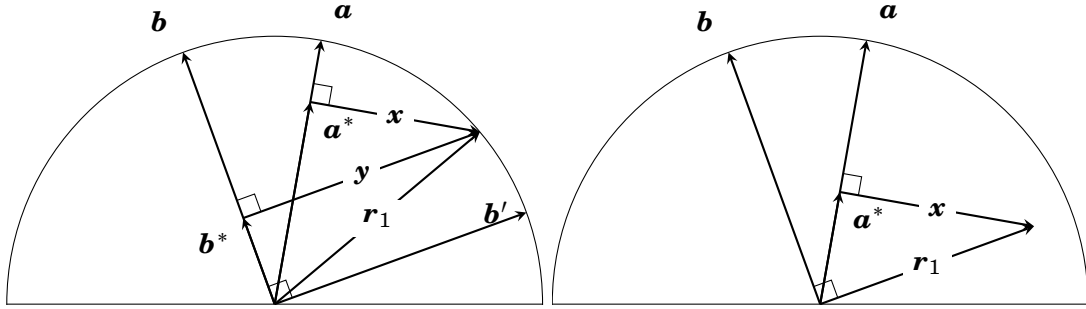
(a) Upper bound diagram. Note that $\boldsymbol{x} \cdot \boldsymbol{y} = \boldsymbol{a} \cdot \boldsymbol{b} \|\boldsymbol{x}\| \|\boldsymbol{y}\|$.

(b) Upper bound diagram version where $\Delta A \geq \boldsymbol{a} \cdot \boldsymbol{b}$. Here we can achieve the (trivial) upper bound of $\Delta B = 1$ since $\boldsymbol{r} \cdot \boldsymbol{b} = 0$. Note that if one wants to have ρ a pure state one can obtain this by moving perpendicularly out of the $\boldsymbol{a}, \boldsymbol{b}$ plane.

Figure 3.6: Illustration of the $\boldsymbol{r}_1$ vectors which maximize $\Delta_\rho B = \|\boldsymbol{y}\|$ given a fixed $\Delta_\rho A = \|\boldsymbol{x}\|$

The presence of an upper bound less than 1 for ΔB in the cases shown in (3.3.18) and (3.3.20) (i.e., $\Delta A < \boldsymbol{a} \cdot \boldsymbol{b}$) can be interpreted in terms of another observable $B' = \boldsymbol{b}' \cdot \boldsymbol{\sigma}$ where $\boldsymbol{b}'$ is the unit vector, in the plane spanned by $\boldsymbol{a}$ and $\boldsymbol{b}$, orthogonal to $\boldsymbol{b}$. With this definition we have $\Delta_\rho^2 B = 1 - \Delta_\rho^2 B'$ so the lower bound on the uncertainty $\Delta B'$ (due to its trade-off with ΔA) imposes an upper bound on ΔB.

By solving the various quadratic equations we obtain the following relation which defines, exactly, the allowed uncertainty region. In particular we can achieve our aim of giving a closed form for the minimum and maximum values of $\Delta_\rho B$ given a fixed ΔA. Note that the resulting tight uncertainty relation (3.3.14) is state-independent in the sense described above:

the bounds for $\Delta_\rho^2 B$ depend only on the chosen $\Delta^2 A$ and the observables A and B.

3.3.3 Schrödinger uncertainty relation

We now turn to a brief analysis of the Schrödinger inequality, beginning with the following observation.

Lemma 3.2. *The identity* (3.3.15) *for unit vectors* $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3$ *and any vector* $\boldsymbol{r} \in \mathbb{R}^3$ *can be rewritten in the following two equivalent forms:*

(3.3.26)
$$\|\boldsymbol{a} \times \boldsymbol{b}\|^2 \|\boldsymbol{r}\|^2 = \big((\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{r}\big)^2 + \big\|(\boldsymbol{a} \times \boldsymbol{b}) \times \boldsymbol{r}\big\|^2$$

(3.3.27)
$$\iff \big(1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2\big) + \big(1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2\big) + \big(\|\boldsymbol{a} \times \boldsymbol{b}\|^2 - (\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2\big) = \|\boldsymbol{a} \times \boldsymbol{b}\|^2 \big(1 - \|\boldsymbol{r}\|^2\big) + 2(1 - \boldsymbol{a} \cdot \boldsymbol{b}\, \boldsymbol{a} \cdot \boldsymbol{r}\, \boldsymbol{b} \cdot \boldsymbol{r})$$

(3.3.28)
$$\iff \big(1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2\big)\big(1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2\big) - \big((\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2 + (\boldsymbol{a} \cdot \boldsymbol{b} - \boldsymbol{a} \cdot \boldsymbol{r}\, \boldsymbol{b} \cdot \boldsymbol{r})^2\big) = \|\boldsymbol{a} \times \boldsymbol{b}\|^2 \big(1 - \|\boldsymbol{r}\|^2\big).$$

Proof. Recall the identity based on the Lagrange formula for the double vector product,

(3.3.29)
$$\|(\boldsymbol{a} \times \boldsymbol{b}) \times \boldsymbol{r}\|^2 = \|\boldsymbol{a}(\boldsymbol{b} \cdot \boldsymbol{r}) - \boldsymbol{b}(\boldsymbol{a} \cdot \boldsymbol{r})\|^2 = (\boldsymbol{a} \cdot \boldsymbol{r})^2 + (\boldsymbol{b} \cdot \boldsymbol{r})^2 - 2(\boldsymbol{a} \cdot \boldsymbol{b})(\boldsymbol{a} \cdot \boldsymbol{r})(\boldsymbol{b} \cdot \boldsymbol{r}).$$

We use this to rewrite (3.3.15) as follows:

(3.3.30)
$$\|\boldsymbol{a} \times \boldsymbol{b}\|^2 \|\boldsymbol{r}\|^2 = (\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2 + (\boldsymbol{a} \cdot \boldsymbol{r})^2 + (\boldsymbol{b} \cdot \boldsymbol{r})^2 - 2\boldsymbol{a} \cdot \boldsymbol{b}\, \boldsymbol{a} \cdot \boldsymbol{r}\, \boldsymbol{b} \cdot \boldsymbol{r}$$

(3.3.31)
$$= \|\boldsymbol{a} \times \boldsymbol{b}\|^2 - \big(\|\boldsymbol{a} \times \boldsymbol{b}\|^2 - (\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2\big) +$$
$$1 - \big(1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2\big) + 1 - \big(1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2\big) - 2(\boldsymbol{a} \cdot \boldsymbol{b})(\boldsymbol{a} \cdot \boldsymbol{r})(\boldsymbol{b} \cdot \boldsymbol{r})$$

Upon rearranging terms, we obtain (3.3.27), showing at once its equivalence with (3.3.15).

Next, working on the left hand side of (3.3.28), we obtain:

(3.3.32)
$$\big(1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2\big)\big(1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2\big) - \big((\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2 + (\boldsymbol{a} \cdot \boldsymbol{b} - \boldsymbol{a} \cdot \boldsymbol{r}\, \boldsymbol{b} \cdot \boldsymbol{r})^2\big)$$

(3.3.33)
$$= 1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2 - (\boldsymbol{b} \cdot \boldsymbol{r})^2 + (\boldsymbol{a} \cdot \boldsymbol{r})^2 (\boldsymbol{b} \cdot \boldsymbol{r})^2 - (\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2$$
$$- (\boldsymbol{a} \cdot \boldsymbol{b})^2 - (\boldsymbol{a} \cdot \boldsymbol{r})^2 (\boldsymbol{b} \cdot \boldsymbol{r})^2 + 2\boldsymbol{a} \cdot \boldsymbol{b}\, \boldsymbol{a} \cdot \boldsymbol{r}\, \boldsymbol{b} \cdot \boldsymbol{r}$$

(3.3.34)
$$= \big(1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2\big) + \big(1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2\big) - 1 + \big(\|\boldsymbol{a} \times \boldsymbol{b}\|^2 - (\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2\big)$$
$$- \big(\|\boldsymbol{a} \times \boldsymbol{b}\|^2 + (\boldsymbol{a} \cdot \boldsymbol{b})^2\big) + 2\boldsymbol{a} \cdot \boldsymbol{b}\, \boldsymbol{a} \cdot \boldsymbol{r}\, \boldsymbol{b} \cdot \boldsymbol{r}$$

(3.3.35)
$$= \big(1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2\big) + \big(1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2\big) + \big(\|\boldsymbol{a} \times \boldsymbol{b}\|^2 - (\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2\big)$$
$$- 2(1 - \boldsymbol{a} \cdot \boldsymbol{b}\, \boldsymbol{a} \cdot \boldsymbol{r}\, \boldsymbol{b} \cdot \boldsymbol{r}) =: g(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{r})$$

Equating this with the right hand side of (3.3.28), we see that (3.3.28) implies (3.3.27).

Conversely, we may use (3.3.27) to see that $g(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{r})$ is actually equal $\|\boldsymbol{a} \times \boldsymbol{b}\|^2 \big(1 - \|\boldsymbol{r}\|^2\big)$, which shows that (3.3.27) implies (3.3.28). ∎

We recall that for any qubit state $\rho = \frac{1}{2}(I + \boldsymbol{r} \cdot \boldsymbol{\sigma})$ we have

$$(3.3.36) \qquad \Delta_\rho^2 A = 1 - (\boldsymbol{a} \cdot \boldsymbol{r})^2, \quad \Delta_\rho^2 B = 1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2,$$

$$(3.3.37) \qquad \left| \langle [A, B] \rangle_\rho \right| = 2 \left| (\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{r} \right|,$$

$$(3.3.38) \qquad \langle AB + BA \rangle_\rho = 2(\boldsymbol{a} \cdot \boldsymbol{b}), \quad \langle A \rangle_\rho = \boldsymbol{a} \cdot \boldsymbol{r}, \quad \langle B \rangle_\rho = \boldsymbol{b} \cdot \boldsymbol{r}.$$

Further, we note that the variance of the observable $C = \boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{\sigma}$ is $\Delta_\rho^2 C = \|\boldsymbol{a} \times \boldsymbol{b}\|^2 - (\boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{r})^2$. This can be used to translate the above identities into two equivalent forms of uncertainty equations.

Theorem 3.3. *The observables* $A = \boldsymbol{a} \cdot \boldsymbol{\sigma}$, $B = \boldsymbol{b} \cdot \boldsymbol{\sigma}$, *and* $C = \boldsymbol{a} \times \boldsymbol{b} \cdot \boldsymbol{\sigma}$ *obey the following equivalent uncertainty equations for all states* $\rho = \frac{1}{2}(I + \boldsymbol{r} \cdot \boldsymbol{\sigma})$:

$$(3.3.39) \qquad \Delta_\rho^2 A + \Delta_\rho^2 B + \Delta_\rho^2 C = \|\boldsymbol{a} \times \boldsymbol{b}\|^2 (1 - \|\boldsymbol{r}\|^2) + 2(1 - \boldsymbol{a} \cdot \boldsymbol{b} \, \boldsymbol{a} \cdot \boldsymbol{r} \, \boldsymbol{b} \cdot \boldsymbol{r}),$$

$$(3.3.40) \qquad \Delta_\rho^2 A \Delta_\rho^2 B - \left[\frac{1}{4} \left| \langle [A, B] \rangle_\rho \right|^2 + \frac{1}{4} \left(\langle AB + BA \rangle_\rho - 2 \langle A \rangle_\rho \langle B \rangle_\rho \right)^2 \right] = \|\boldsymbol{a} \times \boldsymbol{b}\|^2 (1 - \|\boldsymbol{r}\|^2).$$

This yields, in particular, the Schrödinger inequality (3.1.2).

The Schrödinger inequality does not have the form of a state-independent uncertainty relation, except in the case $\boldsymbol{a} \cdot \boldsymbol{b} = 0$ (treated in Subsection 3.3.1). Nevertheless, it does provide a specification of the lower boundary of the uncertainty relation. The upper boundary is obtained by appliciation of the full equation (3.3.40).

Corollary 3.1. *The upper and lower boundary value of each vertical segment* $\{(\Delta A, \Delta_\rho B) \mid \rho \in \mathscr{S}(\Delta A)\}$ *of the uncertainty region for* $A = \boldsymbol{a} \cdot \boldsymbol{\sigma}, B = \boldsymbol{b} \cdot \boldsymbol{\sigma}$ *is determined by the Schrödinger bound*

$$(3.3.41) \qquad S(A, B, \rho) = \frac{1}{4} \left| \langle [A, B] \rangle_\rho \right|^2 + \frac{1}{4} \left(\langle AB + BA \rangle_\rho - 2 \langle A \rangle_\rho \langle B \rangle_\rho \right)^2$$

as follows:

$$(3.3.42) \qquad \Delta^2 B_{min} = \min \left\{ \left. \frac{S(A, B, \rho)}{\Delta^2 A} \right| \rho \in \mathscr{S}(\Delta A) \right\},$$

$$(3.3.43) \qquad \Delta^2 B_{max} = \max \left\{ \left. \frac{S(A, B, \rho)}{\Delta^2 A} \right| \rho \in \mathscr{S}(\Delta A) \right\}.$$

Proof. This is a direct consequence of Eq. (3.3.40) and the fact that the maximizing and minimizing states can be chosen to be pure. ∎

Thus we find that the strengthening (3.3.40) of the Schrödinger inequality into an equation determines the uncertainty region for $\boldsymbol{a} \cdot \boldsymbol{\sigma}$, $\boldsymbol{b} \cdot \boldsymbol{\sigma}$. However, the Schrödinger inequality itself gives the lower bound for $\Delta_\rho B$ given ΔA, and similarly the lower bound for ΔA given $\Delta_\rho B$. Since the uncertainty region is symmetric under reflection on the axis $\Delta A = \Delta B$, the minimal

boundaries for the two uncertainties together, obtained by the Schrödinger inequality alone, determine the uncertainty region.

An unexpected feature becomes apparent in the case of minimal uncertainty. Note that one may always move the vector $\boldsymbol{r}$ into the plane spanned by $\boldsymbol{a}$ and $\boldsymbol{b}$ without changing the variances $\Delta_\rho^2 A$ and $\Delta_\rho^2 B$. Since $\boldsymbol{r}$ is then perpendicular to $\boldsymbol{a} \times \boldsymbol{b}$ the "commutator term" $((\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{r})^2$ in the uncertainty relation (3.3.40) is zero for all of these vectors. Hence the lower uncertainty bound (which is always assumed on unit vectors, so that the above corollary remains applicable) is a feature purely of the anti-commutator term. This term is analogous in form to the classical covariance; however, in the quantum context, this interpretation only applies where the observables are compatible and thus have physical joint probabilities.

3.3.4 Uncertainty region for triples of ±1-valued qubit observables

Here, as before, $A = \boldsymbol{a} \cdot \boldsymbol{\sigma}$ and $B = \boldsymbol{b} \cdot \boldsymbol{\sigma}$, for $\boldsymbol{a}, \boldsymbol{b}$ non-collinear 3-vectors of unit norm, however we now consider the uncertainty region $\mathrm{PUR}_\Delta(A, B, C)$, where $C = \boldsymbol{c} \cdot \boldsymbol{\sigma}$, for $\boldsymbol{c} = \frac{\boldsymbol{a} \times \boldsymbol{b}}{\|\boldsymbol{a} \times \boldsymbol{b}\|}$. We summarise this uncertainty region in theorem 3.4.

Theorem 3.4. *Given* $\Delta^2 C \in [0, 1]$*, then*

$$(3.3.44) \qquad \sqrt{1 - \Delta^2 C} \le \Delta^2 A \le 1,$$

and

$$(3.3.45) \qquad \xi_- \le \Delta^2 B \le \begin{cases} \xi_+ & \Delta^2 A \le 1 - \Delta^2 C \|\boldsymbol{a} \times \boldsymbol{b}\|^2 \\ 1 & otherwise \end{cases}$$

where

$$(3.3.46)$$
$$\xi_\pm = (\boldsymbol{a} \cdot \boldsymbol{b})^2 \Delta^2 A + \|\boldsymbol{a} \times \boldsymbol{b}\|^2 (1 - \Delta^2 A + 1 - \Delta^2 C) \pm 2(\boldsymbol{a} \cdot \boldsymbol{b}) \sqrt{1 - \Delta^2 A} \|\boldsymbol{a} \times \boldsymbol{b}\| \sqrt{\Delta^2 A + \Delta^2 C - 1}.$$

Furthermore this inequality is tight, that is it determines exactly the set of variances that make up the uncertainty region.
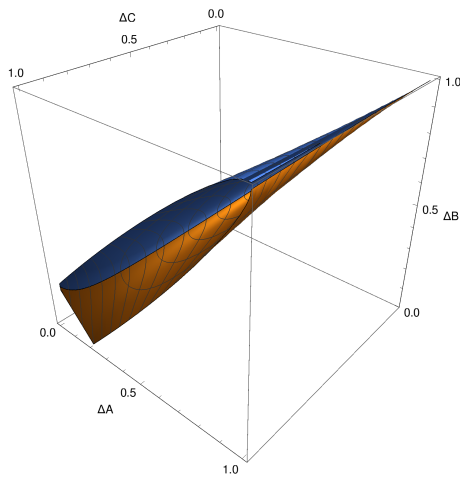
(a) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{\pi}{16}$.
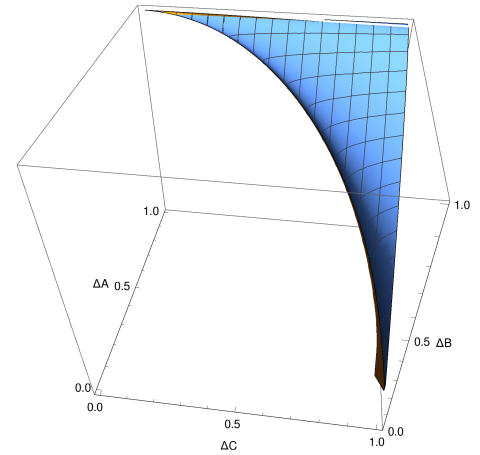
(b) Another view of the uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{\pi}{16}$.
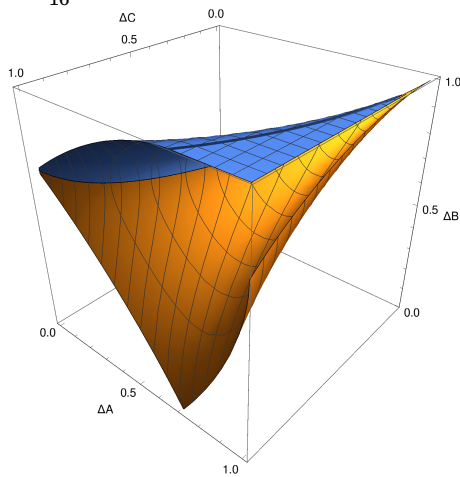
(c) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{4\pi}{16}$.
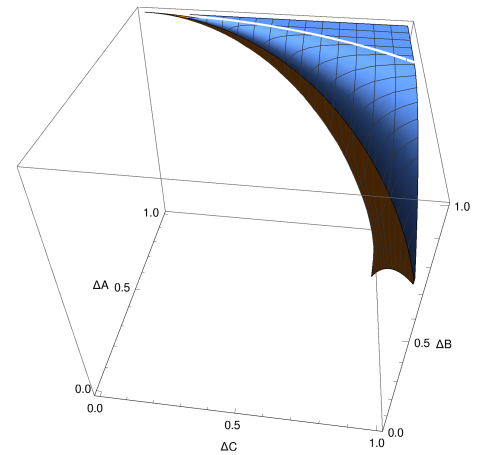
(d) Another view of the uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{4\pi}{16}$.
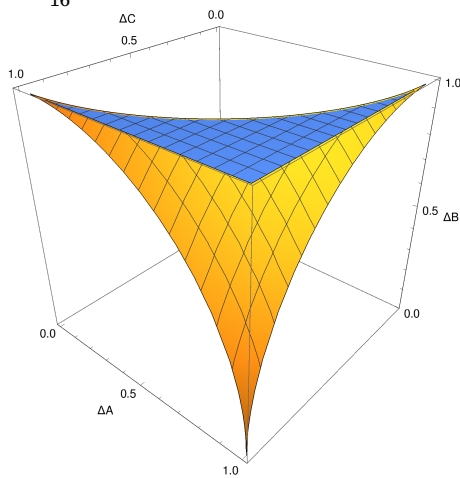
(e) The uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{8\pi}{16}$.
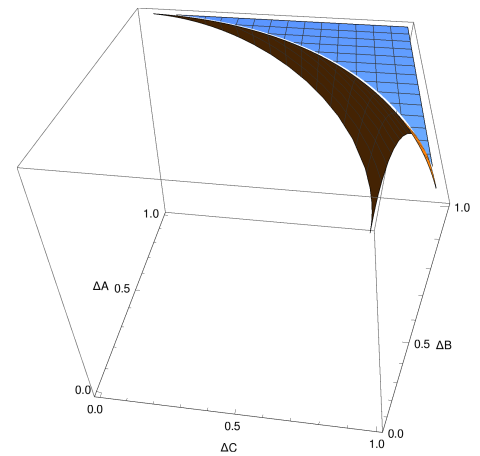
(f) Another view of the uncertainty region with $\boldsymbol{a} \cdot \boldsymbol{b} = \cos \frac{8\pi}{16}$.

Figure 3.7: Plots of the uncertainty region for 3 sharp, ±1-valued qubit observables where the Bloch vector of one observable is orthogonal to the other two.

Proof. Without loss of generality, we assume the following

$$(3.3.47) \qquad \boldsymbol{a} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad\qquad \boldsymbol{b} = \begin{pmatrix} b_1 \\ b_2 \\ 0 \end{pmatrix} \qquad\qquad \boldsymbol{c} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$(3.3.48) \qquad 1 > b_1, b_2 > 0,$$

where we have exploited our freedom to choose coordinates to fix $\boldsymbol{a}$, b_3 and the equivalence of the observables $\boldsymbol{e} \cdot \boldsymbol{\sigma}$ and $-\boldsymbol{e} \cdot \boldsymbol{\sigma}$ to choose b_1, b_2 and $c_3 > 0$. We now choose a $Z \in (0,1)$ and consider the disk formed by the intersection of the Bloch sphere with plane $\{\boldsymbol{r} \in \mathbb{R}^3 \,|\, \boldsymbol{r} \cdot \boldsymbol{c} = Z\}$. This disk is perpendicular to the vector $\boldsymbol{c}$, has centre $Z\boldsymbol{c}$ and radius $\sqrt{1 - Z^2}$. The largest value of r_1 realisable in this disk is $\sqrt{1 - Z^2}$ which, since $\Delta_\rho^2 C = 1 - Z^2$ and $\Delta_\rho^2 A = 1 - r_1^2$ implies (3.3.44).

Fixing $\Delta_\rho^2 C$ in the allowed range defines two lines through the disk, since it implies $|\boldsymbol{a} \cdot \boldsymbol{r}| = \sqrt{1 - \Delta_\rho^2 A}$. We compute the extreme values of r_2 allowed given the constraint that $|\boldsymbol{r}|^2 \leq 1$

$$(3.3.49) \qquad Z^2 + (1 - \Delta_\rho^2 A) + r_2^2 = 1$$

$$(3.3.50) \qquad r_2^2 = \Delta_\rho^2 A - Z^2$$

$$(3.3.51) \qquad r_2 = \pm\sqrt{\Delta_\rho^2 A^2 + \Delta_\rho^2 C^2 - 1},$$

where we note that the constraint (3.3.44) implies that $\Delta_\rho^2 A^2 + \Delta_\rho^2 C^2 \geq 1$. We now seek the values of $\Delta_\rho^2 A$ for which the trivial upper bound $\Delta_\rho^2 B = 1$ is attainable. For this we require

$$(3.3.52) \qquad 0 = \boldsymbol{b} \cdot \boldsymbol{r}$$

$$(3.3.53) \qquad = b_1 r_1 + b_2 r_2$$

$$(3.3.54) \qquad = (\boldsymbol{a} \cdot \boldsymbol{b})\sqrt{1 - \Delta_\rho^2 A} + \|\boldsymbol{a} \times \boldsymbol{b}\| r_2.$$

Combining (3.3.51) and (3.3.54), shows that the least value of $\Delta_\rho^2 A$ for which it is possible to attain $\Delta_\rho^2 B = 1$ is given by

$$(3.3.55) \qquad 0 = (\boldsymbol{a} \cdot \boldsymbol{b})\sqrt{1 - \Delta_\rho^2 A} - \|\boldsymbol{a} \times \boldsymbol{b}\|\sqrt{\Delta_\rho^2 A^2 + \Delta_\rho^2 C^2 - 1}$$

$$(3.3.56) \qquad \|\boldsymbol{a} \times \boldsymbol{b}\|^2 \left(\Delta_\rho^2 A^2 + \Delta_\rho^2 C^2 - 1\right) = (\boldsymbol{a} \cdot \boldsymbol{b})^2 \left(1 - \Delta_\rho^2 A\right)$$

$$(3.3.57) \qquad \Delta_\rho^2 A = 1 - \|\boldsymbol{a} \times \boldsymbol{b}\|^2 \Delta_\rho^2 C^2.$$

The minimum attainable value of $\Delta_\rho^2 B$, as well as the maximum attainable in the in the region where $\Delta_\rho^2 A < 1 - \|\boldsymbol{a} \times \boldsymbol{b}\|^2 \Delta_\rho^2 C^2$ are then obtained by substituting the positive and negative extreme values of b_2, respectively into the variance formula $\Delta_\rho^2 B = 1 - (\boldsymbol{b} \cdot \boldsymbol{r})^2$. ∎

3.4 Qutrit uncertainty

3.4.1 Extended qubit observables

A natural continuation of the qubit example is provided by extending the general, sharp, ± 1-valued qubit observables $\boldsymbol{a} \cdot \boldsymbol{\sigma}$ and $\boldsymbol{b} \cdot \boldsymbol{\sigma}$ into a third dimension

$$(3.4.1) \qquad \mathrm{A} = (\boldsymbol{a} \cdot \boldsymbol{\sigma}) \oplus 0 = \begin{pmatrix} \boldsymbol{a} \cdot \boldsymbol{\sigma} & 0 \\ 0 & 0 \end{pmatrix}$$

$$(3.4.2) \qquad \mathrm{B} = (\boldsymbol{b} \cdot \boldsymbol{\sigma}) \oplus 0 = \begin{pmatrix} \boldsymbol{b} \cdot \boldsymbol{\sigma} & 0 \\ 0 & 0 \end{pmatrix},$$

where $\boldsymbol{a}$ and $\boldsymbol{b}$ are normalised, and $\boldsymbol{\sigma}$ is the usual vector of qubit Pauli matrices. It is easily verified that given any qutrit density matrix we can attain the same variance pairs $\Delta^2 \mathrm{A}, \Delta^2 \mathrm{B}$ with a density matrix of the form

$$(3.4.3) \qquad \rho = \frac{w}{2}(\mathrm{I}_2 + \boldsymbol{r} \cdot \boldsymbol{\sigma}) \oplus (1 - w) = \begin{pmatrix} \frac{w}{2}(\mathrm{I}_2 + \boldsymbol{r} \cdot \boldsymbol{\sigma}) & 0 \\ 0 & (1-w) \end{pmatrix},$$

where $\frac{1}{2}(\mathrm{I}_2 + \boldsymbol{r} \cdot \boldsymbol{\sigma})$ is a qubit density matrix, and w is a real parameter between 0 and 1 (inclusive). We can compute the variances of A and B for a state of this form directly from the definition, to find

$$(3.4.4) \qquad \Delta_\rho^2 \mathrm{A} = w - w^2 (\boldsymbol{a} \cdot \boldsymbol{r})^2$$

$$(3.4.5) \qquad \Delta_\rho^2 \mathrm{B} = w - w^2 (\boldsymbol{b} \cdot \boldsymbol{r})^2.$$

Unfortunately an analytical description of the uncertainty region does not seem to be forthcoming for the case of general $\boldsymbol{a}$ and $\boldsymbol{b}$, although numerical approximations to the boundary curve may readily be computed. We therefore focus our attention on the case $\boldsymbol{a} \cdot \boldsymbol{b} = 0$. We note that projecting a vector onto the plane spanned by $\boldsymbol{a}$ and $\boldsymbol{b}$ leaves both of variances unchanged so, without loss of generality, set

$$(3.4.6) \qquad \boldsymbol{r} = r_a \boldsymbol{a} + r_b \boldsymbol{b},$$

subject to

$$(3.4.7) \qquad r_a^2 + r_b^2 \le 1.$$

At a fixed w the minimum for $\Delta_\rho^2 \mathrm{B}$ will be attained by making $(\boldsymbol{b} \cdot \boldsymbol{r})^2$ as large as possible; we therefore set $r_b^2 = 1 - r_a^2$. We also see that for $X \in [0,1]$ the equation $X = \Delta_\rho^2 \mathrm{A}$ enforces a relation between w and r_a^2:

$$(3.4.8) \qquad w_\pm = \frac{1 \pm \sqrt{1 - 4X r_a^2}}{2 r_a^2}.$$

Since w is required to be real for ρ to be a valid state, we need $r_a^2 \leq \frac{1}{4X}$; in addition w must be in the range $[0,1]$. Note that $w_+ \geq w_- \geq 0$, so that w_- leads to a valid state whenever w_+ does. Now, $w_+ \leq 1$ is equivalent to having both $r_a^2 \geq \frac{1}{2}$ and $r_a^2 \geq 1 - X$. Denoting

$$(3.4.9) \qquad Y_\pm = w_\pm - w_\pm^2(1 - r_a^2),$$

we have that

$$(3.4.10) \qquad Y_+ - Y_- = \left(2r_a^2 - 1\right)\frac{\sqrt{1 - 4Xr_a^2}}{r_a^4}.$$

Hence, wherever w_+ leads to a valid quantum state, w_- gives a lower $\Delta_\rho^2 B$, and so we can focus on w_-, Y_-. The requirement $w_- \leq 1$ is satisfied if and only if $r_a^2 \leq 1 - X$ whenever $r_a^2 < \frac{1}{2}$. We now note that $w_-(r_a^2)$ always gives a valid solution when $r_a^2 = 0$,

$$(3.4.11) \qquad w_-(0) = \lim_{r_a^2 \to 0} \frac{1 - \sqrt{1 - 4Xr_a^2}}{2r_a^2} = X,$$

$$(3.4.12) \qquad Y_-(0) = X(1 - X),$$

It is easily verified that $w_-(r_a^2) \equiv w_-(u) > X$ whenever $u = r_a^2 > 0$; this entails that the derivative

$$(3.4.13) \qquad w_-'(u) = \frac{w_-(u) - X}{u\sqrt{1 - 4Xu}} > 0 \quad \text{for } u > 0.$$

We then differentiate $Y_-(u)$

$$(3.4.14) \qquad Y_-'(u) = \frac{2(w_- - X)(1 - w_-)}{u\sqrt{1 - 4Xu}} \geq 0,$$

so that $Y_-(r_a^2) - Y_-(0) \geq 0$ always. Hence we take $r_a^2 = 0$ to find the minimum $\Delta^2 B_{\min} = X(1 - X)$ at a fixed $\Delta^2 A = X$. The lower boundary of the uncertainty region is therefore given by the curve $\Delta B = \Delta A\sqrt{1 - \Delta^2 A}$. Since the region is symmetric under reflection on the axis $\Delta A = \Delta B$ and in the present case must contain the uncertainty region for orthogonal qubit observables, it is given by the set

$$(3.4.15) \quad \mathrm{PUR}_\Delta(A, B) = \left\{(\Delta A, \Delta B) \in [0,1] \times [0,1] \,\middle|\, \Delta B \geq \Delta A\sqrt{1 - \Delta^2 A} \text{ and } \Delta A \geq \Delta B\sqrt{1 - \Delta^2 B}\right\},$$

shown in Figure 3.8.

3.4.1.1 "Gell-Mann" observables

An interesting counterpoint to section 3.3.2 is provided by the case of quantum observables on a three dimensional Hilbert space. Here it is possible to show, by counterexample, that
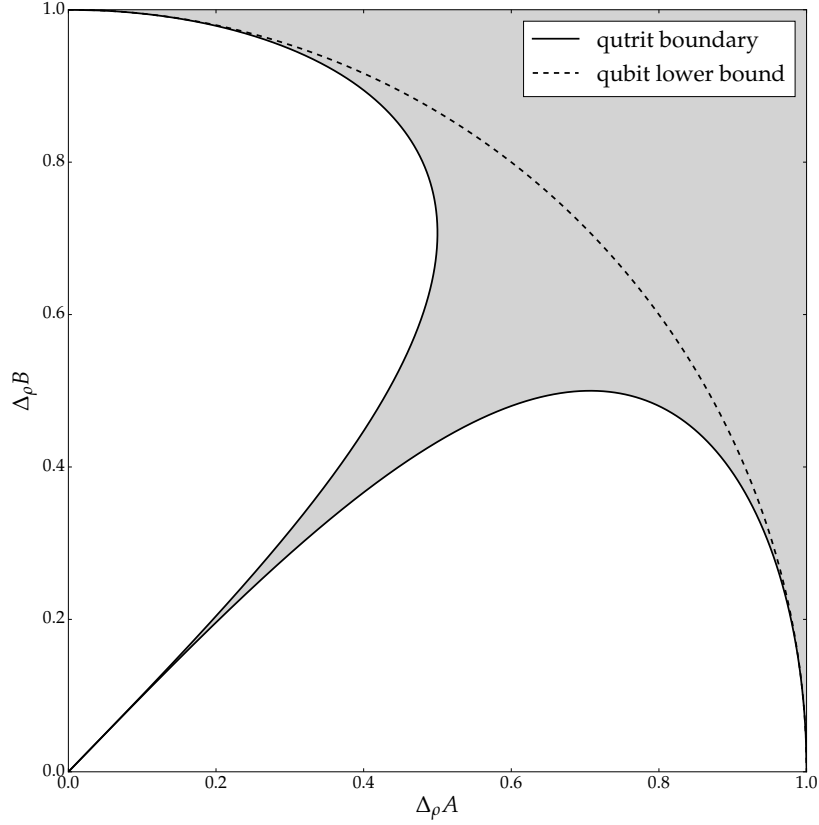
Figure 3.8: The uncertainty region for the qutrit observables defined in equation (3.4.1). The dashed line indicates the lower boundary of the set of standard deviation pairs achievable by states of the form $\rho_2 \oplus 0$, where ρ_2 is a qubit density matrix. The points $(0,1)$, $(0,0)$ and $(1,0)$ are attained by the states $\frac{1}{2}(\mathrm{I}_2 + \boldsymbol{b} \cdot \boldsymbol{\sigma}) \oplus 0$, $0 \oplus 1$, and $\frac{1}{2}(\mathrm{I}_2 + \boldsymbol{a} \cdot \boldsymbol{\sigma}) \oplus 0$ respectively. The "spike" towards the origin is formed by putting increasingly more of the weight of the state in the shared eigenspace of the two operators.

the Schrödinger uncertainty relation is not sufficient to define the exact uncertainty region. We expect that the same will hold true for all finite dimensions greater than two. For our counterexample we choose the observables to be two of the Gell-Mann matrices, and let ρ be an arbitrary, Hermitian, positive-semi-definite three by three matrix of trace 1.

$$(3.4.16) \qquad A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \rho = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{12}^* & \rho_{22} & \rho_{23} \\ \rho_{13}^* & \rho_{23}^* & \rho_{33} \end{pmatrix}$$

Then

$$(3.4.17) \qquad \mathbf{A}^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad [\mathbf{A},\mathbf{B}] = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$
$$\mathbf{B}^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathbf{A}\mathbf{B}+\mathbf{B}\mathbf{A} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$(3.4.18) \qquad \langle \mathbf{A} \rangle_\rho = \rho_{11} - \rho_{22}$$

$$(3.4.19) \qquad \langle \mathbf{B} \rangle_\rho = \rho_{13} + \rho_{13}^* = 2\,\mathrm{Re}\,\rho_{13}$$

$$(3.4.20) \qquad \left\langle \mathbf{A}^2 \right\rangle_\rho = \rho_{11} + \rho_{22}$$

$$(3.4.21) \qquad \left\langle \mathbf{B}^2 \right\rangle_\rho = \rho_{11} + \rho_{33} = 1 - \rho_{22}$$

$$(3.4.22) \qquad \langle [\mathbf{A},\mathbf{B}] \rangle_\rho = \rho_{13} - \rho_{13}^* = 2\,\mathrm{Im}\,\rho_{13}$$

$$(3.4.23) \qquad \langle \mathbf{A}\mathbf{B}+\mathbf{B}\mathbf{A} \rangle_\rho = \rho_{13} + \rho_{13}^* = \langle \mathbf{B} \rangle_\rho$$

$$(3.4.24) \qquad \Delta_\rho^2 \mathbf{A} = \rho_{11} + \rho_{22} - (\rho_{11} - \rho_{22})^2$$

$$(3.4.25) \qquad \Delta_\rho^2 \mathbf{B} = \rho_{11} + \rho_{33} - 4(\mathrm{Re}\,\rho_{13})^2.$$

We can set ρ_{12} and ρ_{23} equal to zero without changing the uncertainties or the Schrödinger relation at all. Note that the new matrix we obtain by this procedure is positive semi-definite and trace 1 if the original was. We can, therefore, explore the entire uncertainty region using states of the form

$$(3.4.26) \qquad \rho = \begin{pmatrix} \rho_{11} & 0 & \rho_{13} \\ 0 & \rho_{22} & 0 \\ \rho_{13}^* & 0 & \rho_{33} \end{pmatrix}.$$

By elementary methods (differentiating, finding local extrema and comparing them) we can find the minimum and maximum values of $\Delta_\rho^2 \mathbf{B}$ as a function of $\Delta_\rho^2 \mathbf{A}$. Because of the way the various constraints change with $\Delta_\rho^2 \mathbf{A}$ the functional form of the minima and maxima also change. In all there are ten distinct bounding curve segments, given in equation (B.1.33) and shown in Figure 3.9. We give a derivation of these curves in Appendix B.1.

Similar to the qubit case, the uncertainty region contains nontrivial upper bounds, and it is not of a simple (e.g. convex shape); however, there are fundamental differences. The region shown in Fig. 3.9 does touch and include the origin (0,0), reflecting the fact that the two observables have a common eigenstate. The shape of the region is also quite asymmetrical; in particular, it is not possible for both uncertainties to get large simultaneously. It is possible that these features can be connected to trade-off relations involving other observables, as we indicated in the qubit case. However, this may require the acquisition of a host of further case
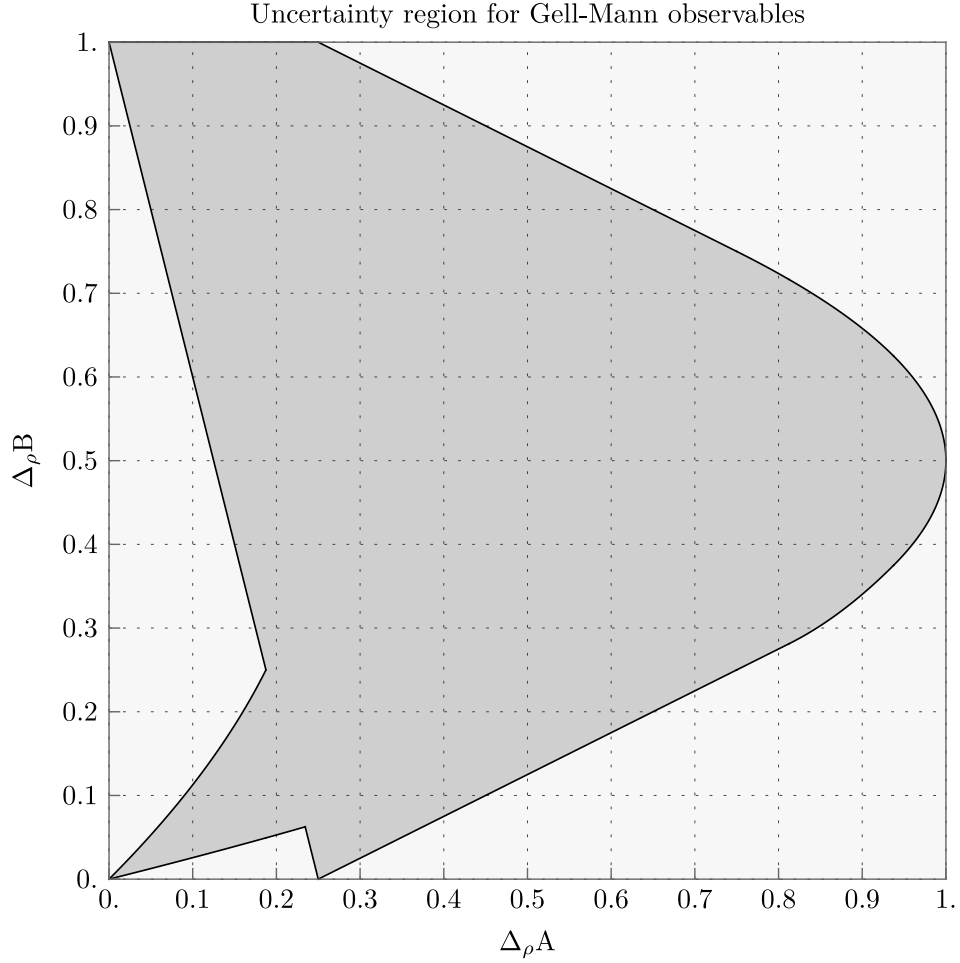
Figure 3.9: The uncertainty region for the qutrit observables defined in equation (3.4.16). The dark region is the allowed uncertainty region.

studies. The Schrödinger relation does not entail the lower bound of the uncertainty region in this case.

We show this by determining the maximum value in the interval of possible values of the Schrödinger bound, $\{S(A, B, \rho) \,|\, \rho \in \mathscr{S}(\Delta A)\}$, and we find indeed that for some range of values of ΔA,

$$(3.4.27) \quad \Delta^2 B_{\min} > \max\left\{ \frac{1}{4\Delta_\rho^2 A} \left(\left| \langle [A, B] \rangle_\rho \right|^2 + \left(\langle AB + BA \rangle_\rho - 2 \langle A \rangle_\rho \langle B \rangle_\rho \right)^2 \right) \right\} = \max\left\{ \frac{S(A, B, \rho)}{\Delta^2 A} \right\}.$$

To verify this we first solve the equation

$$(3.4.28) \qquad\qquad x = \Delta_\rho^2 A$$

$$(3.4.29) \qquad\qquad = 1 - \rho_{33} - \left(2\rho_{11} + \rho_{33} - 1 \right)^2$$

$$(3.4.30) \qquad\qquad \implies \rho_{33}^\pm = \frac{1}{2}\left(1 - 4\rho_{11} \pm \sqrt{1 + 8\rho_{11} - 4x} \right).$$

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We then note that in the range $x \in \left[\frac{3}{4}, 1\right]$ only the ρ_{33}^+ solution with $\rho_{11} \in \left[\frac{1}{2} - \frac{\sqrt{1-x}}{2}, \frac{1}{2} + \frac{\sqrt{1-x}}{2}\right] =: I$ leads to ρ being a valid state (positive and trace 1). We therefore seek

(3.4.31)
$$f(x) := \frac{1}{x} \max\left\{\mathrm{Im}(\rho_{13})^2 + \mathrm{Re}(\rho_{13})^2 \left(6 - 8\rho_{11} - 4\rho_{33}^+\right)^2 \,\middle|\, \rho_{11} \in I, |\rho_{13}|^2 \leq \rho_{11}\rho_{33}^+\right\}$$

(3.4.32)
$$= \frac{1}{x} \max\left\{\mathrm{Im}(\rho_{13})^2 + \mathrm{Re}(\rho_{13})^2 \left(4 - 2\sqrt{1 + 8\rho_{11} - 4x}\right)^2 \,\middle|\, \rho_{11} \in I, |\rho_{13}|^2 \leq \rho_{11}\rho_{33}^+\right\}$$

(3.4.33)
$$= \frac{1}{x} \max\left\{\left(\lambda + (1-\lambda)\left(4 - 2\sqrt{1 + 8\rho_{11} - 4x}\right)^2\right)\frac{\rho_{11}}{2}\left(1 - 4\rho_{11} + \sqrt{1 + 8\rho_{11} - 4x}\right)\,\middle|\, \rho_{11} \in I, \lambda \in [0,1]\right\}.$$

For ease of exposition we here restrict our attention to $x = 1$, in which case only $\rho_{11} = \frac{1}{2}$ leads to a valid quantum state. We can therefore directly compute $f(1) = 0$, and note that as the function is continuous there is an interval where the Schrödinger inequality is too weak to completely describe the uncertainty region.

3.5 Conclusion

We have introduced the notion of the uncertainty region for a pair (or a finite collection) of quantum observables, and provided a range of examples illustrating the concept. In contrast to the well-known uncertainty relations, we observed that an uncertainty region is most appropriately described by a *state-independent* form of relation that describes, in particular, its boundary.

We have given a geometrical derivation of the exact uncertainty region for an arbitrary pair of ±1-valued qubit observables, in the explicit form of a state independent uncertainty relation. When the observables A, B have non-orthogonal Bloch vectors $\boldsymbol{a}, \boldsymbol{b}$, we found non-trivial upper bounds for the variance $\Delta_\rho^2 B$ as a function of $\Delta_\rho^2 A$, and showed that this may be understood in terms of the uncertainty trade-off between A and another observable B' (whose Bloch vector $\boldsymbol{b}'$ is in the plane of $\boldsymbol{a}, \boldsymbol{b}$ and perpendicular to $\boldsymbol{b}$): the observables B, B' obey the uncertainty relation $\Delta^2 B + \Delta^2 B' \geq 1$, and then the minimum value of $\Delta B'$ given ΔA dictates the maximum value of ΔB.

We have seen that the Schrödinger inequality determines the uncertainty region in the qubit case, despite the fact that it is only a state-independent inequality in the case where $\boldsymbol{a} \perp \boldsymbol{b}$. This is essentially due to the fact that satisfaction of this inequality is equivalent to the positivity condition for states.

Finally we described the uncertainty region for two pairs of qutrit observables, which provide illustrations of the often non-trivial shape of an uncertainty region. The pairs of observables studied here do have a common eigenstate and consequently the uncertainty region is allowed to touch and include the point (0,0). The last example also demonstrates the fact

that the Schrödinger relation cannot, in general, determine the lower boundary (and certainly not the upper boundary) of the uncertainty region in dimensions higher than two.

The examples studied here reinforce the qualitative understanding of the uncertainty principle as the statement that the incompatibility (non-commutativity) of a pair of observables generally enforces a state-independent lower bound to their uncertainty region. Where incompatible observables do have joint eigenstates, allowing the uncertainty region to include the origin, one must still expect that parts of some neighbourhood of (0,0) will remain excluded from the uncertainty region.

The structure of uncertainty regions is still unknown. It seems likely that an expanding library of case studies, like those described above, will help point the way for future investigations of this theory. A notable feature of these investigations is how rapidly the computations become more difficult as the Hilbert space dimension increases, for example attempting to generalise the results of sections 3.3.2 and 3.4.1 to the case of extended qubit observables with non-orthogonal Bloch vectors requires computing the roots of fifth order polynomials. One avenue for further investigation could be the use of numerical methods in the analysis; since the variance is quadratic in the state the problem may be reduced to polynomial root finding, which may be efficiently solved using well known numerical techniques. To conclude, we expect that much can be learned about the uncertainty principle through the study of uncertainty regions and hope our investigation will encourage some readers to undertake further case studies.

Infinite dimensional preparation uncertainty

4.1   Introduction

A standard introductory course on quantum mechanics, for example one following ref. [33], [97] or [76], mentions several infinite dimensional state-spaces. Namely the pure states of a particle free to move on an line ($L^2(\mathbb{R})$), a particle fixed to a one dimensional ring ($L^2(\mathbb{T})$, where $\mathbb{T}$ denotes the unit circle), and a particle in a "box", a finite interval (without loss of generality $L^2([-\pi,\pi])$). Preparation uncertainty for position and momentum observables has been studied for several of these spaces, with the variance [41] and Shannon-entropy [9, 8] uncertainty regions for the Euclidean spaces being characterised in 1927 and 1975, respectively. More recently the case of the particle on a ring has been addressed for both measurement uncertainty and preparation uncertainty [13].

There does not seem to have been a similar analysis for the particle in a box system. In part this omission may be due to the lack of phase-space symmetry which makes the problem more tractable in other cases. We contrast our approach with that taken in ref. [58] which seems superficially similar, however the authors of that reference only examine the uncertainty of eigenstates of the Hamiltonian of the "box" system, rather than the full state-space. Our approach is more similar to the original Heisenberg result, in that we seek an uncertainty relation which is valid for all quantum states of the system.

We will be interested in comparing our results to those obtained for the ring, as well as the free particle. A barrier to this is that it is not possible to directly define the variance for a probability distribution defined on a circle. This may be seen by noting that in order to define the variance one must first define the mean and that, for example, the uniform distribution on the circle does not have a well-defined mean. For this reason Busch, Kiukas and Werner employed the α-deviation (see equation (2.5.32)), in order to compare the localisation

of probability distributions.

In section 4.2 we will define the observables of interest, which will be obtained as restrictions of the standard position and momentum observables on $L^2(\mathbb{R})$. We will also determine the relevant domain, the largest subspace of $L^2([-\pi,\pi])$ for which the first and second moments of both observables are finite. In section 4.3 we will determine some constraints on the structure of the uncertainty region, in particular we show that it is the epigraph of a continuous function, which decreases on the interval $\left(0, \frac{\pi^2}{3} - 2\right)$, attains a minimum of $\frac{1}{4}$ at $\frac{\pi^2}{3} - 2$ and increases again on $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$. In addition the boundary function is convex in the interval on which it is increasing. In section 4.4 we obtain some analytical bounds on the boundary function, in particular showing it is bounded below by, and is asymptotic to, the hyperbola which bounds the free particle uncertainty region. In section 4.5 we discuss numerical approximations to the boundary curve, in particular we give a method to approximate a curve which upper bounds the boundary function. We prove that the curve which is being approximated is exactly the boundary function in the region where the latter is convex, and conjecture that this is also true outside this interval. Finally in section 4.6 we compare the results for the box system with those already known for the particle on a ring, and the free particle. We note that the variance for the box system is the same as the 2-deviation used for the analysis of the ring system in [13], so it is reasonable to compare the two.

4.2 State-space

We model the box system as one obtained from the full Hilbert space $L^2(\mathbb{R})$ by imposing the restriction that the states are zero outside the interval $[-\pi,\pi]$, this is an idealisation of the physical situation where there are large (but finite) potential "walls" causing the probability density of the particle to decay rapidly outside the box. There is an obvious isometry $l\colon L^2([-\pi,\pi]) \to L^2(\mathbb{R})$ which extends a state by 0 outside the allowed interval

$$(4.2.1) \qquad (l\varphi)(x) = \begin{cases} \varphi(x), & x \in [-\pi,\pi] \\ 0, & \text{otherwise} \end{cases},$$

from which we obtain position and momentum observables

$$(4.2.2) \qquad \mathbf{E}\colon X \mapsto l^* \mathbf{E}_0(X)l$$

$$(4.2.3) \qquad \mathbf{F}\colon Y \mapsto l^* \mathbf{F}_0(Y)l,$$

where $\mathbf{E}$, $\mathbf{E}$ are the observables (POVMs) acting on $L^2([-\pi,\pi])$ and $\mathbf{E}_0$, $\mathbf{F}_0$ are those for $L^2(\mathbb{R})$, i.e. $\mathbf{E}_0$, $\mathbf{F}_0$ are the spectral measures of the standard position and momentum self-adjoint operators respectively. More explicitly $\mathbf{E}_0(X)$ is the operator which multiplies by the characteristic

function of the (Borel) set X, while $\mathbf{F}_0$ is the Fourier transform

$$(4.2.4) \qquad (\mathbf{E}_0(X)\varphi)(x) = \begin{cases} \varphi(x), & x \in X \\ 0, & \text{otherwise} \end{cases}$$

$$(4.2.5) \qquad (\mathbf{F}_0(Y)\varphi)(x) = (\mathscr{F}^* \mathbf{E}_0(Y)\mathscr{F})(x),$$

where the unitary $\mathscr{F}$ implements the Fourier transform

$$(4.2.6) \qquad (\mathscr{F}\varphi)(p) = \int_{\mathbb{R}} e^{-2\pi i x p} \varphi(x) dx.$$

We restrict our attention to those states for which the first and second moments of both observables are finite, this imposes some non-trivial conditions on the quantum states.

Theorem 4.1. *The first and second moments*

$$(4.2.7) \qquad \langle \mathbf{E}[1] \rangle_\varphi = \int_{\mathbb{R}} x \langle \varphi | \mathbf{E}(dx)\varphi \rangle \qquad\qquad \langle \mathbf{F}[1] \rangle_\varphi = \int_{\mathbb{R}} p \langle \varphi | \mathbf{F}(dp)\varphi \rangle$$

$$(4.2.8) \qquad \langle \mathbf{E}[2] \rangle_\varphi = \int_{\mathbb{R}} x^2 \langle \varphi | \mathbf{E}(dx)\varphi \rangle \qquad\qquad \langle \mathbf{F}[2] \rangle_\varphi = \int_{\mathbb{R}} p^2 \langle \varphi | \mathbf{F}(dp)\varphi \rangle.$$

are finite on the domain of the self-adjoint operator

$$(4.2.9) \qquad \mathscr{D}(\mathbf{F}[1]^* \mathbf{F}[1]) = \left\{ \varphi \in \mathscr{D}(\mathbf{F}[1]) \,\middle|\, \varphi' \text{ is abs. cont.}, \varphi'' \in L^2([-\pi,\pi]) \right\},$$

furthermore they are not finite on any larger domain.

Proof. The actions of the moments are exactly those of the more familiar operators on $L^2(\mathbb{R})$, since they are just restrictions of those operators to $L^2([-\pi,\pi])$, so

$$(4.2.10) \qquad \big(\mathbf{E}[1]\varphi\big)(x) = x\varphi(x) \qquad\qquad \big(\mathbf{F}[1]\varphi\big)(x) = -i\varphi'(x)$$

$$(4.2.11) \qquad \big(\mathbf{E}[2]\varphi\big)(x) = x^2\varphi(x) \qquad\qquad \big(\mathbf{F}[2]\varphi\big)(x) = -\varphi''(x).$$

The states φ must be absolutely continuous, as well as taking the value 0 at the boundary points, $-\pi$ and π, in order that $l\varphi$ is in the domain of $\mathbf{F}_0[1]$. We note that $\mathbf{F}[1]$ is *not* a self-adjoint operator on its domain,

$$(4.2.12) \qquad \mathscr{D}(\mathbf{F}[1]) = \left\{ \varphi \in L^2([-\pi,\pi]) \,\middle|\, \varphi \text{ is abs. cont.}, \varphi' \in L^2([-\pi,\pi]), \varphi(-\pi) = \varphi(\pi) = 0 \right\},$$

and therefore the expectation of the second moment $\mathbf{F}[2]$ is finite on a larger set than

$$(4.2.13) \qquad \mathscr{D}(\mathbf{F}[1]\mathbf{F}[1]) = \left\{ \varphi \in \mathscr{D}(\mathbf{F}[1]) \,\middle|\, \big(\mathbf{F}[1]\varphi\big) \in \mathscr{D}(\mathbf{F}[1]) \right\}.$$

The difference between equations (4.2.13) and (4.2.9) being that in the latter we have the extra condition that $\varphi'(-\pi) = \varphi'(\pi) = 0$. To prove that this is the largest possible domain for $\mathbf{F}[2]$ we recall that the integral of a real function against a POVM is a symmetric operator

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(see, e.g., [14], chapter 4) and that von Neumann's formulas imply that a densely defined self adjoint operator can have no proper symmetric extensions. Indeed any symmetric extension of a densely defined symmetric operator $\mathbf{A}$ is a restriction of $\mathbf{A}^*$ [2].

It remains to show that the domain of $\mathbf{F}[1]^* \mathbf{F}[1]$ is indeed the set given in (4.2.9), which we may verify using integration by parts, recalling that the domain of $\mathbf{F}[1]^*$ is given by the set of vectors ψ such that there exists a vector $\xi \in L^2([-\pi, \pi])$ such that for all $\phi \in \mathscr{D}(\mathbf{F}[1])$

$$(4.2.14) \qquad \langle \psi | \mathbf{F}[1] \phi \rangle = \langle \xi | \phi \rangle.$$

In the position representation we therefore have

$$(4.2.15) \qquad \langle \psi | \mathbf{F}[1] \phi \rangle = \langle \xi | \phi \rangle$$

$$(4.2.16) \qquad \int_{-\pi}^{\pi} dx \, \psi(x)^* (-i) \phi'(x) = \int_{-\pi}^{\pi} dx \, \xi(x)^* \phi(x),$$

$$(4.2.17) \qquad = \Xi(x) \phi(x) \big|_{-\pi}^{\pi} + \int_{-\pi}^{\pi} dx \, i \Xi(x)^* \phi'(x)$$

$$(4.2.18) \qquad = \int_{-\pi}^{\pi} dx \, i \Xi(x)^* \phi'(x),$$

where

$$(4.2.19) \qquad \Xi(x) = \xi(-\pi) + \int_{-\pi}^{x} dy \, \xi(y),$$

exists since we assume $\xi \in L^2([-\pi, \pi])$ and the interval is bounded, while ϕ' exists since we are assuming $\phi \in \mathscr{D}(\mathbf{F}[1])$. A standard argument, choosing ϕ such that ϕ' ranges over a basis for $L^2([-\pi, \pi])$ now ensures that

$$(4.2.20) \qquad \psi(x) = -i \Xi(x)$$

$$(4.2.21) \qquad = -i \xi(-\pi) - i \int_{-\pi}^{x} dy \, \xi(y).$$

There therefore exists a Lebesgue integrable function g such that

$$(4.2.22) \qquad \psi(x) = \psi(-\pi) + \int_{-\pi}^{x} dy \, g(y),$$

by Lebesgue's fundamental theorem of calculus this is equivalent to ψ being absolutely continuous.

We do not require any additional conditions to ensure that the moments of position are finite, since absolute continuity, combined with the boundary conditions, implies that the states are bounded functions in the position representation. $\blacksquare$

Due to the boundary conditions in (4.2.9) we do not have shift operators, which move the states in position space. Explicitly, given a pure state $\varphi \in \mathscr{D}(\mathbf{F}[1]^* \mathbf{F}[1])$, and $a \in [0, 2\pi]$ the

function

(4.2.23)
$$\tilde{\varphi} : [-\pi, \pi] \to \mathbb{C}$$

(4.2.24)
$$\tilde{\varphi} : x \mapsto \begin{cases} \varphi(x+a), & x+a \in [-\pi, \pi] \\ \varphi(x+a-2\pi), & x+a-2\pi \in [-\pi, \pi] \end{cases},$$

will generally *not* obey the boundary conditions and therefore will not be a state. This ability to shift states is a key point in proofs of the usual Heisenberg uncertainty relation for the particle on the line. In particular on the real line one can shift any state in order to set the expectation values of position and momentum to zero, at which point the variance functional becomes linear in the state, offering a significant simplification.

We do, however, have the ability to shift the expectation of the first moment of momentum of the states as we choose.

Lemma 4.1. *Given $\varphi \in \mathscr{D}(\mathrm{F}[1]^* \mathrm{F}[1])$ and $a \in \mathbb{R}$ there exists $\varphi_a \in \mathscr{D}(\mathrm{F}[1]^* \mathrm{F}[1])$ such that*

(4.2.25)
$$\langle \mathrm{E}[1] \rangle_{\varphi_a} = \langle \mathrm{E}[1] \rangle_\varphi \qquad\qquad \langle \mathrm{F}[1] \rangle_{\varphi_a} = \langle \mathrm{F}[1] \rangle_\varphi + a$$

(4.2.26)
$$\langle \mathrm{E}[2] \rangle_{\varphi_a} = \langle \mathrm{E}[2] \rangle_\varphi \qquad\qquad \langle \mathrm{F}[2] \rangle_{\varphi_a} = \langle \mathrm{F}[2] \rangle_\varphi + 2a \langle \mathrm{F}[1] \rangle_\varphi + a^2.$$

Further, these formulae imply that

(4.2.27)
$$\Delta^2_{\varphi_a} \mathrm{E} = \Delta^2_\varphi \mathrm{E}$$

(4.2.28)
$$\Delta^2_{\varphi_a} \mathrm{F} = \Delta^2_\varphi \mathrm{F}.$$

Proof. Given $\varphi \in \mathscr{D}(\mathrm{F}[1]^* \mathrm{F}[1])$ and $a \in \mathbb{R}$ the map

(4.2.29)
$$M_a : \mathscr{D}(\mathrm{F}[1]^* \mathrm{F}[1]) \to \mathscr{D}(\mathrm{F}[1]^* \mathrm{F}[1])$$

(4.2.30)
$$(M_a \varphi) : x \mapsto e^{iax} \varphi(x),$$

leaves the variance of momentum unchanged, along with the expectation of all the moments of position. As required M_a changes the expectation of the first moment of momentum by a

(4.2.31)
$$\langle \mathrm{E}[1] \rangle_{M_a \varphi} = \langle \mathrm{E}[1] \rangle_\varphi \qquad\qquad \langle \mathrm{F}[1] \rangle_{M_a \varphi} = \langle \mathrm{F}[1] \rangle_\varphi + a$$

(4.2.32)
$$\langle \mathrm{E}[2] \rangle_{M_a \varphi} = \langle \mathrm{E}[2] \rangle_\varphi \qquad\qquad \langle \mathrm{F}[2] \rangle_{M_a \varphi} = \langle \mathrm{F}[2] \rangle_\varphi + 2a \langle \mathrm{F}[1] \rangle_\varphi + a^2.$$

These formulae may be proved by expressing the states in the position representation and computing

(4.2.33)
$$(\mathrm{E}[1] M_a \varphi)(x) = -i \frac{d}{dx} \left(e^{iax} \varphi(x) \right)$$

(4.2.34)
$$= e^{iax} \left(a\varphi(x) - i\varphi'(x) \right),$$

and

$$(4.2.35) \qquad (\mathrm{E}[2]M_a\varphi)(x) = -\frac{d^2}{dx^2}\left(e^{iax}\varphi(x)\right)$$

$$(4.2.36) \qquad = -i\frac{d}{dx}e^{iax}\left(a\varphi(x) - i\varphi'(x)\right)$$

$$(4.2.37) \qquad = e^{iax}\left(a^2\varphi(x) - 2ai\varphi'(x) - \varphi''(x)\right),$$

before computing the integrals that form the inner products. ∎

4.3 Structure of the uncertainty region

We are interested in the region

$$(4.3.1) \qquad U = \left\{(\Delta_\rho^2\mathrm{E}, \Delta_\rho^2\mathrm{F}))\big|\rho \in \mathscr{S}\right\},$$

where $\mathscr{S}$ is the set of density operators over the $\mathscr{D}(\mathrm{F}[1]^*\mathrm{F}[1])$, that is the set of operators of the form

$$(4.3.2) \qquad \sum_k p_k P_k,$$

such that the P_k are mutually orthogonal projectors onto subspaces of $\mathscr{D}(\mathrm{F}[1]^*\mathrm{F}[1])$, $p_k \geq 0$ and

$$(4.3.3) \qquad \sum_k p_k = 1.$$

For convenience we summarise the results of this section in proposition 4.1.

Proposition 4.1. *The uncertainty region U is the epigraph of a function $b : (0, \pi^2) \to \mathbb{R}$. Further*

1. *b is continuous.*

2. *b has a global minimum $b(x) \geq b\left(\frac{\pi^2}{3} - 2\right) = \frac{1}{4}$.*

3. *The minimum is unique.*

4. *The minimum is achieved by the state $\psi_0 : x \mapsto \frac{1}{\sqrt{\pi}}\sin\left(\frac{1}{2}(x - \pi)\right)$.*

5. *b is decreasing on $\left(0, \frac{\pi^2}{3} - 2\right)$ and increasing on $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$.*

6. *b is convex on the interval $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$.*

It is clear that the region is contained in the quadrant with $0 \leq \Delta_\rho^2\mathrm{E}$, $0 \leq \Delta_\rho^2\mathrm{P}$, further, since the interval is bounded above and below by π and $-\pi$, we must have that $\Delta_\rho^2\mathrm{E} \leq \langle\mathrm{E}[2]\rangle_\rho \leq \pi^2$. These bounds are classical, for example the probability distribution which assigns probability $\frac{1}{2}$ to each of the points $-\pi$ and π has (classical) position variance π^2.

Lemma 4.2. *For any $x \in (0, \pi^2)$ there exists a state $\varphi \in \mathscr{D}(\mathrm{F}[1]^* \mathrm{F}[1])$ such that*

$$(4.3.4) \qquad\qquad \Delta_\varphi^2 \mathrm{E} = x.$$

Proof. Take any smooth, L^2 normalised, function $f : \mathbb{R} \to \mathbb{R}$, supported only on $[0, 1]$, and consider

$$(4.3.5) \qquad\qquad g_{a,s}(x) = \frac{1}{\sqrt{2s}} f\left(\frac{x-a}{s}\right) + \frac{1}{\sqrt{2s}} f\left(\frac{-x-a}{s}\right),$$

where a is non-negative, s is positive and they are taken such that $a + s < \pi$. The resulting $g_{a,s}$ is a smooth function supported on $[-a-s, -a] \cup [a, a+s]$, with $\langle \mathrm{Q} \rangle_{g_{a,s}} = 0$, and so has finite momentum variance as well as

$$(4.3.6) \qquad\qquad a^2 < \Delta^2 \mathrm{Q} g_{a,s} < (a+s)^2.$$

By varying a and s in the allowed region we see that in any interval $I = (\alpha, \alpha + \varepsilon) \subset (0, \pi^2)$ there exists some state φ with $\Delta_\varphi^2 \mathrm{E} \in I$. Further, given any two position uncertainties $\Delta_\varphi^2 \mathrm{E}$ and $\Delta_\psi^2 \mathrm{Q}$, achieved by pure states φ and ψ we can define the state

$$(4.3.7) \qquad\qquad \xi_\theta = \frac{1}{\sqrt{1 + 2\cos\theta \sin\theta \operatorname{Re}(\langle \varphi | \psi \rangle)}} (\cos\theta\, \varphi + \sin\theta\, \psi),$$

and the continuous, real valued function $\theta \mapsto \Delta_{\xi_\theta}^2 \mathrm{Q}$. The intermediate value theorem then asserts that for every variance $v \in (\Delta_\varphi^2 \mathrm{Q}, \Delta_\psi^2 \mathrm{Q})$ there exists $\theta^* \in (0, \pi)$ such that $\Delta_{\xi_{\theta^*}}^2 \mathrm{Q} = v$. ∎

Lemma 4.3. *Given a state φ with variances $(\Delta_\varphi^2 \mathrm{E}, \Delta_\varphi^2 \mathrm{F})$ the half-line*

$$(4.3.8) \qquad\qquad L = \left\{ (\Delta_\varphi^2 \mathrm{E}, y) \,\middle|\, y \geq \Delta_\varphi^2 \mathrm{F} \right\},$$

is contained in the uncertainty region.

Proof. We apply the map

$$(4.3.9) \qquad\qquad M_a : \varphi \mapsto \left(x \mapsto \varphi(x) e^{aix^2} \right),$$

to obtain a new state, for which the expectations and variances can be computed

$$(4.3.10) \qquad \langle \mathrm{E}[1] \rangle_{M_a \varphi} = \langle \mathrm{E}[1] \rangle_\varphi \qquad\qquad \langle \mathrm{F}[1] \rangle_{M_a \varphi} = \langle \mathrm{F}[1] \rangle_\varphi + 2a \langle \mathrm{E}[1] \rangle_\varphi$$

$$(4.3.11) \qquad \langle \mathrm{E}[2] \rangle_{M_a \varphi} = \langle \mathrm{E}[2] \rangle_\varphi \qquad\qquad \langle \mathrm{F}[2] \rangle_{M_a \varphi} = \langle \mathrm{F}[2] \rangle_\varphi + 4a^2 \langle \mathrm{E}[2] \rangle_\varphi$$

$$(4.3.12) \qquad \Delta_{M_a \varphi}^2 \mathrm{E} = \Delta_\varphi^2 \mathrm{E} \qquad\qquad \Delta_{M_a \varphi}^2 \mathrm{F} = \Delta_\varphi^2 \mathrm{F} + 4a^2 \Delta_\varphi^2 \mathrm{E} - 2a \langle \mathrm{E}[1] \rangle_\varphi \langle \mathrm{F}[1] \rangle_\varphi.$$

Since $0 < \Delta_\varphi^2 \mathrm{E}$ for all states φ there exists an a such that $\Delta_{M_a \varphi}^2 \mathrm{F} = y$, for all $y \geq \Delta_\varphi^2 \mathrm{F}$. ∎

This offers a convenient description of the uncertainty region in terms of a boundary function.

Lemma 4.4. *The uncertainty region is the epigraph (the set of points lying above the graph) of the function*

(4.3.13)
$$b : (0, \pi^2) \to \mathbb{R}$$

(4.3.14)
$$b : x \mapsto \inf \left\{ \Delta_\varphi^2 \mathbf{F} \,\middle|\, \Delta_\varphi^2 \mathbf{E} = x \right\}.$$

Loosely this means that in addition to being unbounded above the uncertainty region has no "holes" in it.

Proof. In order to define such a function it is necessary that for each $x \in (0, \pi^2)$ the infimum in equation (4.3.14) exists and is finite. This is true since the set the infimum is being taken over is non-empty (by lemma 4.2) and bounded below (by 0, since the variance is non-negative).

The uncertainty region U contains the epigraph of b if all the points above b are in U, which follows from lemma 4.3 combined with the definition of b. If (x, y) is a point not in U then there is no point directly below[1] (x, y) which is in U due to lemma 4.3, therefore y is a lower bound for the set

(4.3.15)
$$U(x) = \left\{ \Delta_\varphi^2 \mathbf{F} \,\middle|\, \Delta_\varphi^2 \mathbf{E} = x \right\}.$$

From the definition of $b(x)$ have $y \leq b(x)$, since y is a lower bound for $U(x)$ and $b(x)$ is the greatest lower bound for $U(x)$, so (x, y) is not in the epigraph of b.

Conversely the epigraph of b contains U, which can be seen by noting that for each $x \in (0, \pi^2)$, all of the points (x, y) in the uncertainty region are, by definition directly above $b(x)$. ∎

We can find the minimum of b.

Lemma 4.5. *For all $x \in (0, \pi^2)$*

(4.3.16)
$$b \left(\frac{\pi^2}{3} - 2 \right) = \frac{1}{4} \leq b(x).$$

Further this minimum is achieved by the state

(4.3.17)
$$\psi_0 = \frac{1}{\sqrt{\pi}} \sin \left(\frac{1}{2}(x - \pi) \right),$$

and is unique

(4.3.18)
$$x \neq \frac{\pi^2}{3} - 2 \implies \frac{1}{4} < b(x).$$

Proof. We first seek the least eigenvalue of the self-adjoint operator $\mathbf{F}[2] = \mathbf{F}[1]^* \mathbf{F}[1]$. It is well known that the solutions to

(4.3.19)
$$-\varphi'' = \lambda \varphi$$

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[1] By directly below (resp. above) (x, y) we here mean a point (x, y') such that $y' < y$ (resp. $y' > y$).

are sines and cosines. Applying the boundary conditions $\varphi(-\pi) = \varphi(\pi) = 0$ implies that the eigenstates are

$$(4.3.20) \qquad \psi_k(x) = \frac{1}{\sqrt{\pi}} \sin\left(\frac{k+1}{2}(x-\pi)\right), \qquad k \in \{0,1,2,\dots\}$$

and the eigenvalues are

$$(4.3.21) \qquad \mathbf{F}[2]\psi_k(x) = \frac{(k+1)^2}{4}\psi_k(x),$$

where we have chosen the form such that ψ_k is an odd function if k is odd, and even if k is even. Note that each eigenspace is one-dimensional, in particular there is only one state (up to phase) attaining the value $\langle \mathbf{F}[2] \rangle_{\psi_0} = \frac{1}{4}$. One can compute

$$(4.3.22) \qquad \langle \mathbf{F}[1] \rangle_{\psi_k} = -i\int_{-\pi}^{\pi} dx\,\psi_k(x)^* \psi_k'(x)$$

$$(4.3.23) \qquad = -i\frac{k+1}{2\pi}\int_{-\pi}^{\pi} dx \sin\left(\frac{k+1}{2}(x-\pi)\right)\cos\left(\frac{k+1}{2}(x-\pi)\right)$$

$$(4.3.24) \qquad = 0,$$

so applying lemma 4.1 the least eigenvalue of $\mathbf{F}[2]$ is exactly the least possible momentum variance,

$$(4.3.25) \qquad \inf\left\{\Delta_\rho^2 \mathbf{F} \,\middle|\, \rho \in \mathscr{D}(\mathbf{F}[2])\right\} = \frac{1}{4}.$$

We also compute the position variance of the state ψ_0 which minimises the momentum variance

$$(4.3.26) \qquad \Delta_{\psi_0}^2 \mathbf{E} = \langle \mathbf{E}[2] \rangle_{\psi_0} - \langle \mathbf{E}[1] \rangle_{\psi_0}^2$$

$$(4.3.27) \qquad = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\,x^2 \sin\left(\frac{1}{2}(x-\pi)\right)^2 - \left(\frac{1}{\pi}\int_{-\pi}^{\pi} dx\,x \sin\left(\frac{1}{2}(x-\pi)\right)^2\right)^2$$

$$(4.3.28) \qquad = \frac{\pi^2}{3} - 2.$$

Finally we show the minimum is unique. Assume a state achieves

$$(4.3.29) \qquad \Delta_\varphi^2 \mathbf{F} = \frac{1}{4},$$

then we can employ lemma 4.1 to obtain a state ξ with

$$(4.3.30) \qquad \langle \mathbf{F}[1] \rangle_\xi = 0$$

$$(4.3.31) \qquad \langle \mathbf{F}[2] \rangle_\xi = \frac{1}{4},$$

the fact that the eigenspaces of $\mathbf{F}[2]$ are one dimensional then implies that

$$(4.3.32) \qquad \xi = \alpha\psi_0,$$

for some complex phase α. Reversing the transformation from the proof of lemma 4.1 then implies that

$$(4.3.33) \qquad\qquad \varphi(x) = \alpha e^{-iax}\psi_0(x),$$

for some $a \in \mathbb{R}$. It follows that

$$(4.3.34) \qquad\qquad \Delta_\varphi^2 F = \Delta_{\psi_0}^2 F = \frac{\pi^2}{3} - 2,$$

and so the minimum of b is unique. ∎

The minimum splits b into two regions, to the left of the minimum b is decreasing and to the right it is increasing.

Lemma 4.6. *The boundary function b is strictly decreasing on $\left(0, \frac{\pi^2}{3} - 2\right)$ and strictly increasing on $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$.*

Proof. Choose $x, y \in \left(0, \frac{\pi^2}{3} - 2\right)$, without loss of generality let $x < y$, and choose a sequence of states ρ_n such that

$$(4.3.35) \qquad\qquad \Delta_{\rho_n}^2 E = x$$
$$(4.3.36) \qquad\qquad \lim_{n\to\infty} \Delta_{\rho_n}^2 F = b(x).$$

Such a sequence exists due to the definition of $b(x)$. Without loss of generality, due to lemma 4.1 choose

$$(4.3.37) \qquad\qquad \langle F[1]\rangle_{\rho_n} = 0.$$

Now we mix these states with the projector onto the minimizer of the momentum variance, $|\psi_0\rangle\langle\psi_0|$, and define the functions

$$(4.3.38) \qquad\qquad f_n : (0,1) \to \mathbb{R}$$
$$(4.3.39) \qquad\qquad f_n : \lambda \to \Delta_{\lambda\rho_n + (1-\lambda)|\psi_0\rangle\langle\psi_0|}^2 E,$$

by continuity, for each $n \in \mathbb{N}$ there exists $\lambda^* \in (0,1)$ such that $f_n(\lambda) = y$. Now by the definition of b we have

$$(4.3.40) \qquad\qquad b(y) \leq \langle F[2]\rangle_{\lambda^*\rho_n + (1-\lambda^*)|\psi_0\rangle\langle\psi_0|}$$
$$(4.3.41) \qquad\qquad = \lambda^* \langle F[2]\rangle_{\rho_n} + (1-\lambda^*)\langle F[2]\rangle_{|\psi_0\rangle\langle\psi_0|}$$
$$(4.3.42) \qquad\qquad < \langle F[2]\rangle_{\rho_n}.$$

Taking the limit $n \to \infty$ of the last inequality gives

$$(4.3.43) \qquad\qquad b(y) \leq b(x),$$

as required. The proof for the increasing region is essentially identical. ∎

We recall that the variance is concave as a function of the (mixed) state.

Lemma 4.7. *Given any observable* $\mathbf{A}$*, if* $\mathscr{S}$ *is the set of density operators for which the first and second moments of* $\mathbf{A}$ *are finite then the map* $v : \mathscr{S} \to \mathbb{R}$*,* $v : \rho \mapsto \Delta_\rho^2 \mathbf{A}$ *is concave.*

Proof. Take $\rho, \sigma \in \mathscr{S}$ with finite first and second moments of $\mathbf{A}$ and choose $\lambda \in (0,1)$ then

$$
0 \le \lambda(1-\lambda)\left(\langle \mathbf{A}\rangle_\rho - \langle \mathbf{A}\rangle_\sigma\right)^2 \tag{4.3.44}
$$

$$
\lambda^2 \langle \mathbf{A}\rangle_\rho^2 + (1-\lambda)^2 \langle \mathbf{A}\rangle_\sigma^2 + 2\lambda(1-\lambda)\langle \mathbf{A}\rangle_\rho \langle \mathbf{A}\rangle_\sigma \le \lambda \langle \mathbf{A}\rangle_\rho^2 + (1-\lambda)\langle \mathbf{A}\rangle_\sigma^2 \tag{4.3.45}
$$

$$
\left(\lambda \langle \mathbf{A}\rangle_\rho + (1-\lambda)\langle \mathbf{A}\rangle_\sigma\right)^2 = \tag{4.3.46}
$$

$$
\langle \mathbf{A}^2\rangle_{\lambda\rho+(1-\lambda)\sigma} - \left(\lambda \langle \mathbf{A}\rangle_\rho + (1-\lambda)\langle \mathbf{A}\rangle_\sigma\right)^2 \ge \lambda\left(\langle \mathbf{A}^2\rangle_\rho - \langle \mathbf{A}\rangle_\rho^2\right) + (1-\lambda)\left(\langle \mathbf{A}\rangle_\sigma^2 - \langle \mathbf{A}\rangle_\sigma^2\right) \tag{4.3.47}
$$

$$
\Delta_{\lambda\rho+(1-\lambda)\sigma}^2 \mathbf{A} \ge \lambda\Delta^2 \mathbf{A}\rho + (1-\lambda)\Delta^2 \mathbf{A}\sigma. \tag{4.3.48}
$$

$\blacksquare$

Lemma 4.8. *If* $(v,w),(x,y) \in U$ *and* $v < x$*, and* $w < y$ *then*

$$
\lambda(v,w) + (1-\lambda)(x,y) \in U, \tag{4.3.49}
$$

for all $\lambda \in (0,1)$*.*

Proof. We choose density operators ρ, σ such that

$$
\Delta_\rho^2 \mathbf{E} = v \qquad\qquad \Delta_\sigma^2 \mathbf{E} = x \tag{4.3.50}
$$

$$
\Delta_\rho^2 \mathbf{F} = w \qquad\qquad \Delta_\sigma^2 \mathbf{F} = y \tag{4.3.51}
$$

$$
\langle \mathbf{F}[1]\rangle_\rho = 0 \qquad\qquad \langle \mathbf{F}[1]\rangle_\sigma = 0, \tag{4.3.52}
$$

Consider the real, continuous function

$$
f : \lambda \mapsto \Delta_{\lambda\rho+(1-\lambda)\sigma}^2 \mathbf{E}. \tag{4.3.53}
$$

By continuity, for any $\lambda \in (0,1)$ there exists $\mu \in (0,1)$ such that

$$
f(\mu) = \lambda v + (1-\lambda)x. \tag{4.3.54}
$$

Due to the concavity of the variance functional (lemma 4.7) f is concave and

$$
f(\mu) \ge \mu v + (1-\mu)x \tag{4.3.55}
$$

$$
\lambda v + (1-\lambda)x \ge \mu v + (1-\mu)x \tag{4.3.56}
$$

$$
\lambda(v-x) \ge \mu(v-x) \tag{4.3.57}
$$

$$
\implies \lambda \le \mu. \tag{4.3.58}
$$

Then $w < y$ implies

$$(4.3.59) \qquad \mu w + (1-\mu)y \le \lambda w + (1-\lambda)y.$$

Since we chose ρ and σ such that the first moments of momentum are zero, the momentum variance is linear in the state and

$$(4.3.60) \qquad \Delta^2_{\mu\rho+(1-\mu)\sigma}\mathbf{E} = \mu w + (1-\mu)y$$

$$(4.3.61) \qquad \qquad \qquad \le \lambda w + (1-\lambda)y.$$

Recall we are attempting to show that the point $\lambda(v,w) + (1-\lambda)(x,y) \in U$, but we have now shown that the point $(\lambda v + (1-\lambda)x, \mu w + (1-\mu)y) \in U$, and $\mu w + (1-\mu)y < \lambda w + (1-\lambda)y$. We can now employ lemma 4.3 to move directly up in the uncertainty region to get to the desired point. $\blacksquare$

Lemma 4.9. *The boundary function b is convex on $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$.*

Proof. The boundary function b is convex on this interval iff the restriction of the uncertainty region

$$(4.3.62) \qquad U_> = \left\{(x,y) \in U \,\middle|\, x > \frac{\pi^2}{3} - 2\right\},$$

is convex. We therefore have to show that for any two points $(v,w),(x,y) \in U_>$ the points

$$(4.3.63) \qquad \lambda(v,w) + (1-\lambda)(x,y) \in U,$$

for all $\lambda \in (0,1)$. Without loss of generality we choose $v < x$, we wish to employ lemma 4.8 but we do not necessarily have $w < y$. We therefore consider a new point $(v,w') \in U_>$, directly below (v,w). Since we have shown in lemma 4.6 that the boundary curve is increasing in this interval we can choose $w' \le y$. By lemma 4.8 we have that

$$(4.3.64) \qquad \lambda(v,w') + (1-\lambda)(x,y) \in U.$$

Employing lemma 4.3 and noting that $w' < w \implies \lambda w' + (1-\lambda)y < \lambda w + (1-\lambda)y$ proves that $\lambda w + (1-\lambda)y$ is in the uncertainty region as required. $\blacksquare$

A useful feature of the particle on a line is the ability to rescale states, if $\varphi \in L^2(\mathbb{R})$, and $a > 0$ then

$$(4.3.65) \qquad \varphi_a : x \mapsto \sqrt{a}\varphi ax,$$

is also a state. We do not have this symmetry in the particle in a box system, since "broadening" a state will generally break the boundary conditions, but we can "squeeze" states if we wish.

Lemma 4.10. *If $\varphi \in \mathscr{D}(\mathbf{E}[2])$, $a \geq 1$ and*

$$(4.3.66) \qquad \varphi_a : x \mapsto \begin{cases} \sqrt{a}\varphi(ax), & |ax| \leq \pi \\ 0, & otherwise \end{cases},$$

then $\varphi_a \in \mathscr{D}(\mathbf{E}[2])$, further

$$(4.3.67) \qquad \Delta_{\varphi_a}^2 \mathbf{E} = \frac{1}{a^2} \Delta_\varphi^2 \mathbf{E}$$

$$(4.3.68) \qquad \Delta_{\varphi_a}^2 \mathbf{F} = a^2 \Delta_\varphi^2 \mathbf{F}.$$

Proof. It is well known that this rescaling preserves the domains of the moments of the position and momentum observables on $L^2(\mathbb{R})$. The only additional constraint in the present case is the imposition of the boundary conditions, which are easily shown to be preserved. One can verify equations (4.3.67) and (4.3.68) by directly computing the integrals. ∎

Lemma 4.11. *The boundary function b is continuous.*

Proof. Convex functions are continuous, so b is automatically continuous on $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$. In order to show that b is continuous on $\left(0, \frac{\pi^2}{3} - 2\right)$ we recall that b is decreasing in this interval (lemma 4.6), that monotone functions have limits from the left and the right at every point, and can only have jump discontinuities.

We assume that there exists some discontinuity at a point $a \in \left(0, \frac{\pi^2}{3} - 2\right)$ so that

$$(4.3.69) \qquad \lim_{x \to a^-} b(x) = \lim_{x \to a^+} b(x) + \alpha,$$

where monotonicity implies $\alpha > 0$. We choose a sequence of states ρ_n such that

$$(4.3.70) \qquad \lim_{n \to \infty} \Delta_{\rho_n}^2 \mathbf{E} = x$$

$$(4.3.71) \qquad \Delta_{\rho_n}^2 \mathbf{E} \geq a$$

$$(4.3.72) \qquad \lim_{n \to \infty} \Delta_{\rho_n}^2 \mathbf{F} = \lim_{x \to a^+} b(x).$$

We fix $y < a$ then apply the "squeezing map" from lemma 4.10 to each ρ_n to obtain a sequence of states σ_n such that

$$(4.3.73) \qquad \Delta_{\sigma_n}^2 \mathbf{E} = y,$$

then

$$(4.3.74) \qquad \Delta_{\sigma_n}^2 \mathbf{E} \Delta_{\sigma_n}^2 \mathbf{F} = \Delta_{\rho_n}^2 \mathbf{E} \Delta_{\rho_n}^2 \mathbf{F}$$

$$(4.3.75) \qquad y b(y) \leq \Delta_{\rho_n}^2 \mathbf{E} \Delta_{\rho_n}^2 \mathbf{F},$$

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since, by definition, $b(y) \le \Delta^2_{\sigma_n} F$. Taking the limit $n \to \infty$ on the right hand side then gives the second inequality of

$$(4.3.76) \qquad\qquad y \lim_{x \to a^+} b(x) \le y b(y) \le a \lim_{x \to a^+} b(x),$$

where the first inequality is just the monotonicity of b. Now taking the limit $y \to a^-$ gives

$$(4.3.77) \qquad\qquad a \lim_{x \to a^+} b(x) \le a \lim_{y \to a^-} b(y) \le a \lim_{x \to a^+} b(x),$$

so $\lim_{y \to a^-} b(y) = \lim_{x \to a^+} b(x)$ implying $\lim_{x \to a} b(x)$ exists. A simple generalisation (choosing σ_n such that $\Delta^2_{\sigma_n} E = a$) establishes that $\lim_{y \to a} b(y) = b(a)$.

It remains to show that b is continuous at the point $a = \frac{\pi^2}{3} - 2$. This can be achieved by slightly altering the proof of lemma 4.6. We fix $v < \frac{\pi^2}{3} - 2$ and choose a state ρ such that

$$(4.3.78) \qquad\qquad \Delta^2_\rho E = v$$

$$(4.3.79) \qquad\qquad \langle F[1] \rangle_\rho = 0.$$

Then consider the states

$$(4.3.80) \qquad\qquad \sigma(\lambda) = \lambda \rho + (1 - \lambda) |\psi_0\rangle\langle\psi_0|.$$

As before, for each $x \in \left(v, \frac{\pi^2}{3} - 2 \right]$ there exists some $\lambda(x)$ such that

$$(4.3.81) \qquad\qquad \Delta^2_{\sigma(\lambda(x))} E = x,$$

then, by construction

$$(4.3.82) \qquad\qquad \frac{1}{4} \le b(x) \le \Delta^2_{\sigma(\lambda(x))} F$$

$$(4.3.83) \qquad\qquad = \lambda(x) \Delta^2_\rho F + (1 - \lambda(x)) \Delta^2_{|\psi_0\rangle\langle\psi_0|} F.$$

Now as $x \to a^-$ we have $\lambda \to 0^+$ and obtain

$$(4.3.84) \qquad\qquad \frac{1}{4} \le \lim_{x \to a^-} b(x) \le \frac{1}{4}.$$

The proof for $x \to a^+$ is similar. ∎

4.4 Analytical bounds on the boundary function

We first note that a simple bound may be obtained by recalling that the position and momentum observables E, F we have defined are essentially restrictions of the standard position and momentum observables on $L^2(\mathbb{R})$. In particular given a state $\varphi \in \mathscr{D}(F)$ there exists a state $(l\varphi) \in L^2(\mathbb{R})$ such that

$$(4.4.1) \qquad \langle E[1] \rangle_\varphi = \langle E_0[1] \rangle_{l\varphi} \qquad\qquad \langle E[2] \rangle_\varphi = \langle E_0[2] \rangle_{l\varphi}$$

$$(4.4.2) \qquad \langle F[1] \rangle_\varphi = \langle F_0[1] \rangle_{l\varphi} \qquad\qquad \langle F[2] \rangle_\varphi = \langle F_0[2] \rangle_{l\varphi},$$

where $\mathbf{E}_0, \mathbf{F}_0$ are the position and observables on $L^2(\mathbb{R})$, respectively. This means that the lower bound

$$\Delta_\varphi^2 \mathbf{E} \Delta_\varphi^2 \mathbf{F} \geq \frac{1}{4}, \tag{4.4.3}$$

due to Heisenberg, is still valid for the box system. We can not expect that the Heisenberg bound will be tight for the box, since it is saturated by Gaussian states and these certainly do not obey the boundary conditions $\varphi(-\pi) = \varphi(\pi) = 0$. We can compare this lower bound to upper bounds obtained by considering families of states in $\mathscr{D}(\mathbf{F})$. An obvious family of states is achieved by squeezing the minimizer of momentum, to obtain the bounds

$$\frac{1}{4x} \leq b(x) \leq \frac{1}{4x}\left(\frac{\pi^2}{3} - 2\right), \tag{4.4.4}$$

valid for $x \in \left(0, \frac{\pi^2}{3} - 2\right)$.

Lemma 4.12. *As the position variance becomes small the boundary function b is asymptotic to the canonical hyperbola, that is*

$$\lim_{x \to 0} x b(x) = \frac{1}{4}. \tag{4.4.5}$$

Proof. An upper bound for b, may be computed using the family of "tempered-Gaussians"

$$\xi_s = \frac{1}{N^2} e^{-sx^2}(\pi - x)(x + \pi), \tag{4.4.6}$$

where

$$N = \frac{\sqrt{2\pi}\left(16\pi^4 s^2 - 8\pi^2 s + 3\right)\mathrm{erf}\left(\sqrt{2s}\pi\right) + 4\pi e^{-2\pi^2 s}\left(4\pi^2 s - 3\right)\sqrt{s}}{32 s^{5/2}}, \tag{4.4.7}$$

normalises the state. Then we have

$$\Delta_{\xi_s}^2 \mathbf{E} = \frac{\sqrt{2\pi}\left(16\pi^4 s^2 - 24\pi^2 s + 15\right)\mathrm{erf}\left(\sqrt{2s}\pi\right) + 4\pi e^{-2\pi^2 s}\left(4\pi^2 s - 15\right)\sqrt{s}}{128 s^{7/2} N} \tag{4.4.8}$$

$$\Delta_{\xi_s}^2 \mathbf{F} = \frac{\sqrt{2\pi}\left(16\pi^4 s^2 + 8\pi^2 s + 7\right)\mathrm{erf}\left(\sqrt{2s}\pi\right) + 4\pi e^{-2\pi^2 s}\left(4\pi^2 s - 7\right)\sqrt{s}}{32 s^{3/2} N}. \tag{4.4.9}$$

These expressions are unfortunately rather unwieldy, but we have

$$\lim_{s \to 0^+} \Delta_{\mathbf{E}}^2 \xi_s = 0, \tag{4.4.10}$$

and one can verify

$$\lim_{s \to 0^+} \Delta_{\mathbf{E}}^2 \xi_s \Delta_{\mathbf{F}}^2 \xi_s = \frac{1}{4}. \tag{4.4.11}$$

Combining this limiting upper bound with the lower bound provided by equation (4.4.3) proves that

$$\lim_{x \to 0} x b(x) = \frac{1}{4}. \tag{4.4.12}$$

$\blacksquare$

4.5 Numerical approximation of b

We can do somewhat better than the analytical bounds from section 4.4 in the interval $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$. Here the uncertainty region is convex, and so may be determined by its convex conjugate. We seek

$$(4.5.1) \qquad c(\alpha) := -b^*(-\alpha) = \inf\left\{ b(x) + \alpha x \,\middle|\, x \in \left(\frac{\pi^2}{3} - 2, \pi^2\right) \right\},$$

where we have introduced the minus signs for later convenience. Substituting the definition of b gives

$$(4.5.2) \qquad c(\alpha) = \inf\left\{ \inf\left\{ \Delta_\varphi^2 F \,\middle|\, \Delta_\varphi^2 E = x \right\} + \alpha x \,\middle|\, x \in \left(\frac{\pi^2}{3} - 2, \pi^2\right) \right\}.$$

We notice we can combine the two infima to obtain

$$(4.5.3) \qquad c(\alpha) = \inf\left\{ \Delta_\varphi^2 F + \alpha \Delta_\varphi^2 E \,\middle|\, \varphi \in \mathscr{D}(F[2]) \right\},$$

since searching over all x, and then over all states with variance equal to that x is equivalent to searching over all the states directly. Recalling that b is increasing on $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$, we can see that

$$(4.5.4) \qquad \alpha \geq 0 \implies c(\alpha) = \frac{1}{4} + \alpha\left(\frac{\pi^2}{3} - 2\right).$$

We now employ lemma 4.1 to restrict the search to those states with momentum expectation value equal to 0

$$(4.5.5) \qquad c(\alpha) = \inf\left\{ \langle F[2]\rangle_\varphi + \alpha \Delta_\varphi^2 E \,\middle|\, \varphi \in \mathscr{D}(F[2]), \langle F[1]\rangle_\varphi = 0 \right\}.$$

For convenience we define the function

$$(4.5.6) \qquad h_\alpha : \varphi \mapsto \langle F[2]\rangle_\varphi + \alpha \Delta_\varphi^2 E$$

$$(4.5.7) \qquad = \langle F[2]\rangle_\varphi + \alpha\left(\langle E[2]\rangle_\varphi - \langle F[1]\rangle_\varphi^2\right),$$

and the operator

$$(4.5.8) \qquad H_\alpha = F[2] + \alpha\, E[2],$$

which is self-adjoint on $\mathscr{D}(F[2])$.

Lemma 4.13. *Let $\alpha < 0$ and let η_α be the ground state of H_α. For any state φ*

$$(4.5.9) \qquad \Delta_\varphi^2 E = \Delta_{\eta_\alpha}^2 E \implies \Delta_\varphi^2 F \geq \Delta_{\eta_\alpha}^2 F$$

Proof. First note that H_α commutes with the parity operator

$$\Pi : L^2([-\pi,\pi]) \to L^2([-\pi,\pi]) \tag{4.5.10}$$

$$(\Pi\varphi) : x \mapsto \varphi(-x), \tag{4.5.11}$$

which implies the eigenstates of H_α are also eigenstates of Π, in particular this means that the eigenstates of H_α have zero expectation of position so

$$\Delta_{\mathrm{E}}^2 \eta_\alpha = \langle \mathrm{E}[2] \rangle_{\eta_\alpha}. \tag{4.5.12}$$

Assume there is some state ρ such that

$$\langle \mathrm{E}[2] \rangle_\rho - \langle \mathrm{E}[1] \rangle_\rho^2 = \Delta_\rho^2 \mathrm{E} = \Delta_{\eta_\alpha}^2 \mathrm{E} = \langle \mathrm{E}[2] \rangle_{\eta_\alpha} \tag{4.5.13}$$

$$\langle \mathrm{F}[2] \rangle_\rho < \langle \mathrm{F}[2] \rangle_{\eta_\alpha}, \tag{4.5.14}$$

then

$$\langle \mathrm{F}[2] + \alpha \mathrm{E}[2] \rangle_{\eta_\alpha} \le \mathrm{tr}\left(\rho\left(\mathrm{F}[2] + \alpha \mathrm{E}[2]\right)\right) \tag{4.5.15}$$

$$= \langle \mathrm{F}[2] \rangle_\rho + \alpha \langle \mathrm{E}[2] \rangle_\rho \tag{4.5.16}$$

$$= \langle \mathrm{F}[2] \rangle_\rho + \alpha \left(\langle \mathrm{E}[2] \rangle_{\eta_\alpha} + \langle \mathrm{E} \rangle_\rho^2 \right) \tag{4.5.17}$$

$$< \langle \mathrm{F}[2] + \alpha \mathrm{E}[2] \rangle_{\eta_\alpha} + \alpha \langle \mathrm{E} \rangle_\rho^2 \tag{4.5.18}$$

which is an obvious contradiction for $\alpha < 0$, which is the region for which we do not yet know $c(\alpha)$. We conclude that in this region the ground states of the operators H_α explore the boundary curve. ∎

We are now searching for the ground state, and least eigenvalue, of the operator H_α. It is well known that the solutions to

$$H_\alpha \varphi = \lambda \varphi, \tag{4.5.19}$$

are combinations of Whittaker functions or hypergeometric functions [37, 92]. Unfortunately applying the boundary conditions to determine the constants leads to equations which seem impossible to solve in terms of any common functions. We therefore resort to computing a numerical approximation to the ground state. We can compute the matrix elements of the operator H_α in the basis of eigenfunctions of $\mathrm{F}[2]$

$$\langle \psi_j | H_\alpha \psi_k \rangle = \begin{cases} \frac{(k+1)^2}{4} + \alpha\left(\frac{\pi^2}{3} - \frac{2}{(k+1)^2}\right), & j = k \\ 32\alpha \frac{(j+1)(k+1)}{((j+1)^2 - (k+1)^2)^2}, & j+k \text{ is even} \\ 0, & \text{otherwise} \end{cases} \tag{4.5.20}$$

We then fix some $n \in \mathbb{N}$ and numerically determine the eigenvalues and eigenvectors of an $n \times n$ dimensional truncation of the infinite matrix $\langle \psi_j | H_\alpha \psi_k \rangle$. Once we have computed approximate

values of $c(\alpha_i)$ for a large enough set of values α_i we can compute the variances by numerically approximating the derivative

$$(4.5.21) \qquad\qquad c'(\alpha) = \Delta^2_{\eta_\alpha} \mathbf{E}$$

$$(4.5.22) \qquad\qquad c(\alpha) - \alpha c'(\alpha) = \Delta^2_{\eta_\alpha} \mathbf{F}.$$

The resulting curve is plotted in figure 4.1a. We note that in addition to the eigenvalue $c(\alpha)$ we obtain a numerical approximation to the ground state ξ_α of H_α. We can therefore directly compute approximations to the variances $\Delta^2_{\eta_\alpha} \mathbf{E}$, and $\Delta^2_{\eta_\alpha} \mathbf{F}$, this curve is also plotted in figure 4.1a but is indistinguishable to the curve obtained by numerical differentiation. We are interested in the direct computation of the variances since in addition to exactly giving the boundary curve $b(x)$ in the interval $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$ the ground states are upper bounds on the boundary curve everywhere, as all states are, explicitly

$$(4.5.23) \qquad\qquad b\left(\Delta^2_{\eta_\alpha} \mathbf{E}\right) \leq \Delta^2_{\eta_\alpha} \mathbf{F}.$$

This is the reason that the curve is plotted for the entire interval $(0, \pi^2)$. We conjecture that the ground states of H_α are, in fact, optimisers of b globally, rather than just on the interval $\left(\frac{\pi^2}{3} - 2, \pi^2\right)$, in other words we conjecture that the inequality in equation 4.5.23 is an equality. We note that this is implied by a seemingly natural assumption, that among the optimisers of momentum variance for each fixed position variance, there exist those with position expectation equal to zero.

4.6 Comparisons

We have already compared our results for the particle in a box with the well known variance uncertainty relation for the particle on the line. The particle on a line hyperbola is everywhere a lower bound for the boundary function b for the particle in a box. We have also shown that the two curves are asymptotic to each other in the limit as the variance becomes small in lemma 4.12, that is

$$(4.6.1) \qquad\qquad \lim_{x \to 0} \frac{b(x)}{\frac{1}{4x}} = 1.$$

This is quite natural, loosely one would expect that the more concentrated the box states are around the origin, the less the boundary conditions influence them.

We would also like to compare our results with those from the particle on a ring system addressed in ref. [13], in which α-deviations (see definition 2.5.3) are used to quantify the spread of distributions. As shown in lemma 2.3, for probability measures on the reals this quantity is identical to the usual variance. In contrast to the case of the particle on a ring, a probability measure μ defined on the interval $[-\pi, \pi]$ may be considered identical to a probability measure

on $\mathbb{R}$ which is supported only on $[-\pi, \pi]$. We are therefore free to interpret the variances we have been considering in this chapter as 2-deviations, and directly compare them to the 2-deviations computed in ref. [13]. We invite the reader to compare figures 4.1a and 4.1b, depicting the particle in a box, and on a ring, 2-deviation based uncertainty regions, respectively. The particle on the ring system allows momentum eigenstates, with zero momentum variance and maximal position variance, including the state whose position wavefunction is constant. This is in contrast to the particle in a box system, where there is not a state maximising the position variance, but we can approach the maximum of π^2 by sequences of states which are increasingly concentrated at the points $-\pi$ and π. This is since the variance of probability measures on $[\pi, \pi]$ is maximised by the symmetric two point measure concentrated at the end points.
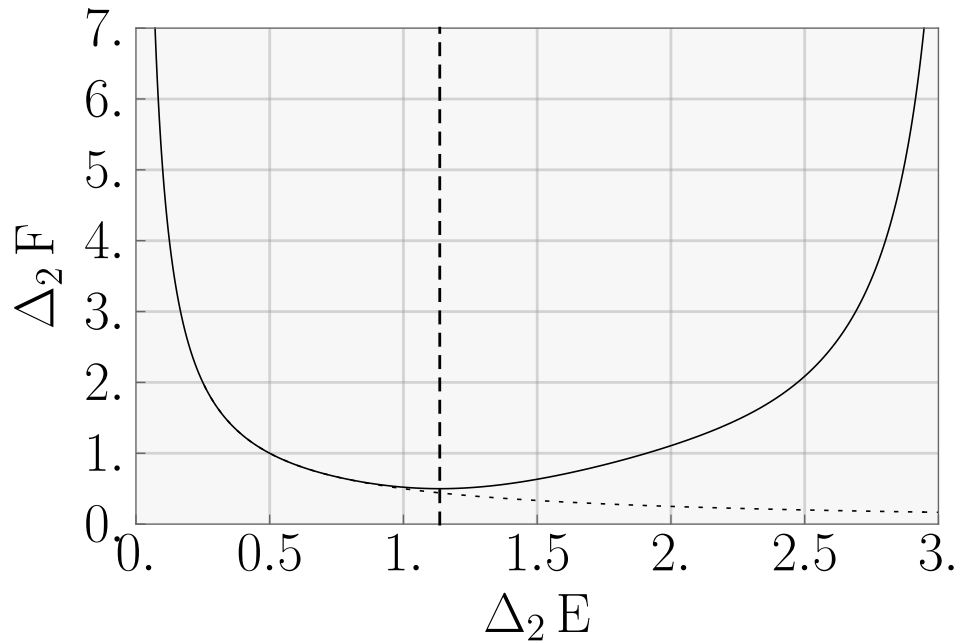
(a) The uncertainty region for the particle in a box system, showing the curve obtained from the least eigenvalues of the operators H_α (solid curve), this is the exact boundary curve on the right hand side of the vertical line at $\sqrt{\frac{\pi^2}{3} - 2}$ (dashed). On the left hand side the true curve lies between the solid curve and the boundary of the free particle uncertainty region (dotted).
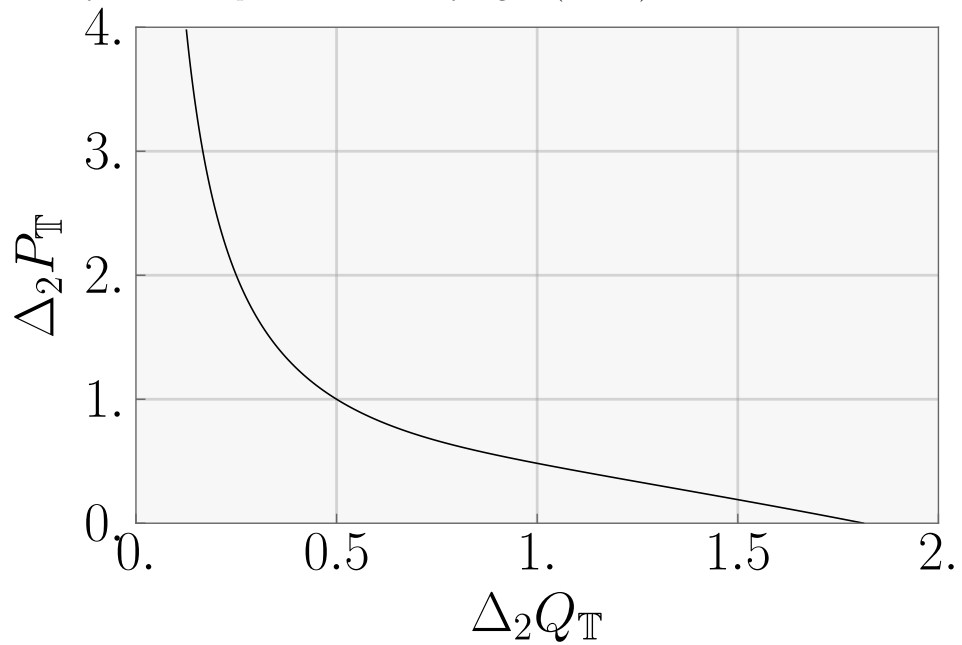
(b) The uncertainty region for the particle on a ring system. Note that this is identical to the top left panel of figure 1 in ref. [13], and is included here only for comparison with figure 4.1a.

Figure 4.1: The box, free particle and ring uncertainty regions.

Part II

Measurement uncertainty

Measurement uncertainty and covariance - finite dimensional case studies

5.1 Introduction

Here we are interested in a scenario where we would like to measure several observables, denoted $\mathbf{E}_i$, to achieve some goal. Unfortunately it may be that these observables are not compatible, that is there is no way to measure them all on the same state. We therefore instead need to measure some compatible observables which are "close", in an appropriate sense, to the targets. The distance measure we use to quantify this closeness will depend on the application, but we will explore methods based based on the p-norm of finite dimensional real vectors below.

The general picture is then summarised in figure 5.1, where $\boldsymbol{E}_i$ are the target observables, and $\boldsymbol{F}_i$ are respective compatible approximations, and $\boldsymbol{J}$ is a joint observable for the $\boldsymbol{F}_i$. If supplied with a "figure of merit" $\boldsymbol{d}$ indicating how well one observable approximates another we can explore the set

$$(5.1.1) \qquad S(\mathbf{E}_1, \mathbf{E}_2 \ldots \mathbf{E}_n) = \{(d(\mathbf{E}_1, \mathbf{F}_1), d(\mathbf{E}_2, \mathbf{F}_2) \ldots d(\mathbf{E}_n, \mathbf{F}_n)) | \mathbf{F}_i \text{ are compatible}\},$$

which we call a *measurement uncertainty region*. We refer to chapter 13 of [14] for an introduction to this line of thinking, and [17, 75] for representative results.

Finding the uncertainty region for generic observables is a difficult problem for interesting figures of merit, with exact results known only in cases with high symmetry or low dimension [96, 27]. Here we do not remedy this situation, but instead employ a systematic approach to exploiting available symmetries to simplify measurement uncertainty problems.

Section 5.2 defines the p-norm based figure of merit used throughout, 5.4 contains some technical lemmas related to how we fill the uncertainty region. Section 5.3 contains quite

general results about the use of covariance to simplify measurement uncertainty problems, with the key result being that if the target observables are covariant, then for every family of jointly measurable approximators there exists a covariant family of joint approximators which is at least as good, according to the d_p figure of merit. Finally sections 5.5 and 5.6 are case studies, applying the previous results to the three mutually unbiased qubit observables, and the pair of observables related by the quantum Fourier transform in dimension n, unknown to us this latter case was addressed already in [90], although our method of proof if different and provides a case study of the use of the invariant mean in solving problems in measurement uncertainty.
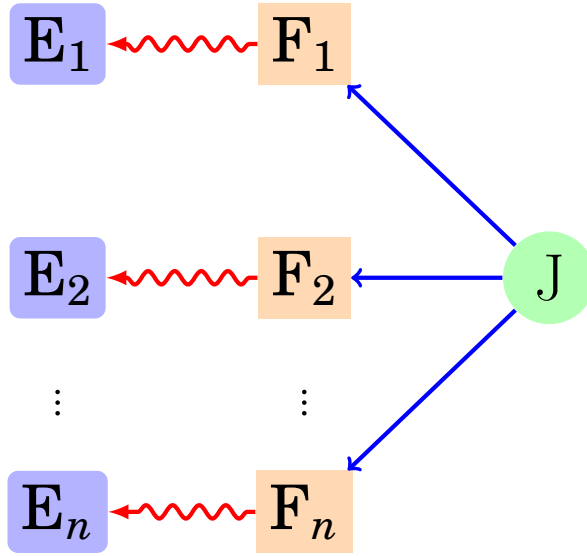
Figure 5.1: Target observables $\mathbf{E}_i$, compatible approximations $\mathbf{F}_i$, and their joint $\mathbf{J}$

5.2 Definitions and error measure

In this chapter we consider separable complex Hilbert spaces and finite outcome observables. A map $\mathbf{E} : \Omega \to \mathscr{L}_s^+(\mathscr{H})$ is an *observable* if it is normalised

$$(5.2.1) \qquad \sum_{\omega \in \Omega} \mathbf{E}(\omega) = \mathbf{I},$$

where $\mathbf{I}$ is the identity operator on $\mathscr{H}$.

A set of n observables on the Hilbert space $\mathscr{H}$, $\{\mathbf{E}_i \mid i = 1 \dots n\}$, with outcome sets Ω_i is *compatible* if there exists a joint observable, $\mathbf{J} : \Omega \to \mathscr{L}_s^+(\mathscr{H})$,

$$(5.2.2) \qquad \sum_{\substack{\boldsymbol{\omega} \in \Omega \\ omega_i = \omega^*}} \mathbf{J}(\boldsymbol{\omega}) = \mathbf{E}_i(\omega^*), \quad \forall i \in 1 \dots n, \ \forall \omega^* \in \Omega_i,$$

where $\Omega = \prod_i \Omega_i$ is the Cartesian product and $\boldsymbol{\omega}_i$ is the ith component of $\boldsymbol{\omega} = (\omega_1, \omega_2 \dots \omega_n)$. Such an observable is called a Cartesian joint observable for the observables $\{\mathbf{E}_i \,|\, i \in 1 \dots n\}$. In other words, $\mathbf{J}$ is a Cartesian joint for the $\mathbf{E}_i$ iff, for each i, $\mathbf{E}_i$ is the ith Cartesian marginal of $\mathbf{J}$.

Given a pair of probability distributions, S and T over the same (finite) set Ω, we can compute the p-norm of their (pointwise) difference. The resulting quantity is a metric on the space of probability distributions over Ω,

$$(5.2.3) \qquad \delta_p(S, T) := \| S - T \|_p$$

$$(5.2.4) \qquad = \left(\sum_{\omega \in \Omega} |S(\omega) - T(\omega)|^p \right)^{\frac{1}{p}}, \quad \forall p \in [1, \infty),$$

$$(5.2.5) \qquad \delta_\infty(S, T) := \max_{\omega \in \Omega} |S(\omega) - T(\omega)|.$$

We note that $\delta_p(S, T) \geq 0$ with equality if and only if $S = T$ and that

$$(5.2.6) \qquad \delta_p(S, T) \leq 2^{\frac{1}{p}}, \quad \forall p \in [1, \infty].$$

When $p = 1$ this quantity is equal to the total variation distance, up to a global factor of 2 and is also equal to the Wasserstein 1-distance between S and T, where the "cost-function" is given by the discrete metric [51, 85].

Given an observable $\mathbf{E} : \Omega \to \mathcal{L}_s^+(\mathcal{H})$ and a quantum state $\rho \in \mathcal{S}(\mathcal{H})$ we can define a probability distribution over Ω,

$$(5.2.7) \qquad \mathbf{E}^\rho : \omega \mapsto \mathrm{tr}\left(\mathbf{E}(\omega)\rho\right).$$

We can lift the distance measure on probability distributions with outcome set Ω to one on observables on the same set, simply by taking the **sup** of the distance for the probability distributions over all states

$$(5.2.8) \qquad d_p(\mathbf{E}, \mathbf{F}) := \sup_{\rho \in \mathcal{S}(\mathcal{H})} \delta_p(\mathbf{E}^\rho, \mathbf{F}^\rho)$$

$$(5.2.9) \qquad = \sup_{\rho \in \mathcal{S}(\mathcal{H})} \left(\sum_{\omega \in \Omega} \left| \mathbf{E}^\rho(\omega) - \mathbf{F}^\rho(\omega) \right|^p \right)^{\frac{1}{p}},$$

where $\mathcal{S}(\mathcal{H})$ is the set of trace 1 density operators within $\mathcal{L}_s^+(\mathcal{H})$. The supremum is finite, because the expression is bounded. We specialise the definition (5.1.1) of the uncertainty region to these error measures, where $\mathbf{E}_i : \Omega_i \to \mathcal{L}_s^+(\mathcal{H})$ are the target observables

(5.2.10)
$$S_p(\mathbf{E}_1, \mathbf{E}_2 \dots \mathbf{E}_n) = \left\{ (d_p(\mathbf{E}_1, \mathbf{F}_1), d_p(\mathbf{E}_2, \mathbf{F}_2) \dots d_p(\mathbf{E}_n, \mathbf{F}_n)) \,\middle|\, \mathbf{F}_i : \Omega_i \to \mathcal{L}_s^+(\mathcal{H}) \text{ are compatible} \right\}, \quad p \in [1, \infty].$$

Given two probability measures μ, ν on the same outcome space $(\Omega, \mathcal{F})$ we say that that μ *dominates* ν if $\mu(X) = 0 \implies \nu(X) = 0$, for all measureable sets $X \in \mathcal{F}$, this is denoted $\mu \gg \nu$. This is often referred to as ν being *absolutely continuous* withe respect to μ.

A theorem due to Radon and Nikodym, [10, 63] states that if μ dominates ν then there exists a μ-measureable function $f : \Omega \to \mathbb{R}$ such that

$$(5.2.11) \qquad \nu(X) = \int_X f \, d\mu,$$

for all $X \in \mathscr{F}$. The f, so defined, is unique up to a set of μ-measure 0, more precisely, if f and g both satisfy (5.2.11) for some measures ν, μ then the set of points $\omega \in \Omega$ such that $f(\omega) \neq g(\omega)$ has μ-measure 0. A function satisfying (5.2.11) is called a (or, by mild abuse of notation the) *Radon-Nikodym derivative* of ν with respect to μ, and denoted $\frac{d\nu}{d\mu}$ so (5.2.11) becomes

$$(5.2.12) \qquad \nu(X) = \int_X \frac{d\nu}{d\mu} \, d\mu.$$

We define the f-divergence, introduced in refs. [3] and [26]. For two probability measures $\mu \gg \nu$, on a measurable space $(\Omega, \mathscr{F})$, and convex function $f : \mathbb{R} \to \mathbb{R}$ such that $f(1) = 0$

$$(5.2.13) \qquad D_f\left(\nu \parallel \mu\right) = \int_\Omega f\left(\frac{d\nu}{d\mu}\right) d\mu.$$

This definition is quite general, and includes several "divergences" well known from the literature. Liese and Vajda [53] express the Kullback–Leibler divergence, Pearson divergence, Hellinger distance and total variation in terms of f-divergences with f equal to

$$(5.2.14) \qquad t \mapsto t \log t,$$

$$(5.2.15) \qquad t \mapsto (t-1)^2,$$

$$(5.2.16) \qquad t \mapsto (\sqrt{t}-1)^2,$$

$$(5.2.17) \qquad t \mapsto |t-1|,$$

respectively, while Arimoto defines the β-divergence, given, for finite outcome sets, by

$$(5.2.18) \qquad t \mapsto \begin{cases} 1 - \max_k p_k, & \beta = 0 \\ \frac{1}{1-\beta}\left(1 - \left(\sum_k p_k^{\frac{1}{\beta}}\right)^\beta\right), & \beta > 0, \text{ and } \beta \neq 1 \\ -\sum_k p_k \log p_k, & \beta = 1 \end{cases}.$$

We note that both the f-divergences and the p-norm based divergences above have the property of *joint convexity*, that is if $\mu_1, \mu_2, \nu_1, \nu_2$ are probability measures such that each divergence is defined, and $\lambda \in [0,1]$ then

$$(5.2.19) \qquad \delta_p(\lambda \nu_1 + (1-\lambda)\nu_2, \lambda \mu_1 + (1-\lambda)\mu_2) \le \lambda \delta_p(\nu_1, \mu_1) + (1-\lambda)\delta_p(\nu_2, \mu_2)$$

$$(5.2.20) \qquad D_f\left(\lambda \nu_1 + (1-\lambda)\nu_2 \parallel \lambda \mu_1 + (1-\lambda)\mu_2\right) \le \lambda D_f\left(\nu_1 \parallel \mu_1\right) + (1-\lambda)D_f\left(\nu_2 \parallel \mu_2\right).$$

The theorems in section 5.3, in particular theorems 5.1 and 5.2, hold for any jointly convex error measure, although they may reduce to trivially stating $\infty \le \infty$ unless the error measure is bounded.

5.3 Invariant Mean

It is useful to embed the set of observables with a fixed outcome set Ω in the real vector space of all maps from Ω to the bounded, self adjoint operators on $\mathcal{H}$ which, for convenience, we denote by $\mathcal{M}$. The set of such maps ranging in the positive operators is a convex cone in $\mathcal{M}$, and the normalisation $\sum_\omega \mathrm{E}(\omega) = \mathrm{I}$ defines an affine space. We equip the space $\mathcal{M}$ with a norm via

$$
(5.3.1) \qquad \|\mathrm{E}\| = \sum_{\omega \in \Omega} \|\mathrm{E}(\omega)\|.
$$

Definition 5.3.1. Given a finite group G, with action $f_g : \Omega \to \Omega$, and normal, completely positive, unital, linear representation R_g acting on $\mathcal{L}_s(\mathcal{H})$ we define the *invariant mean*, $M_{R,f} : \mathcal{M} \to \mathcal{M}$ by

$$
(5.3.2) \qquad M_{R,f}(\mathrm{E})(\omega) = \frac{1}{|G|} \sum_{g \in G} R_{g^{-1}} \big[\mathrm{E}(f_g(\omega)) \big]
$$

which has some useful properties summarised in lemmas 5.1 to 5.3. The invariant mean is motivated by the concept of a group-twirling map, introduced in [30], but the addition of the group action on the outcome set means that the invariant mean of an observable is, in general, different to the observable obtained by acting the twirling map on each of the effects.

Lemma 5.1. *The invariant mean is a norm contraction.*

Proof.

$$
(5.3.3) \qquad \big\| M_{R,f}(\mathrm{E}) \big\| = \sum_{\omega \in \Omega} \big\| M_{R,f}(\mathrm{E})(\omega) \big\|
$$

$$
(5.3.4) \qquad = \sum_{\omega \in \Omega} \left\| \frac{1}{|G|} \sum_{g \in G} R_{g^{-1}} \big[\mathrm{E}(f_g(\omega)) \big] \right\|
$$

$$
(5.3.5) \qquad \leq \sum_{\omega \in \Omega} \frac{1}{|G|} \sum_{g \in G} \big\| R_{g^{-1}} \big[\mathrm{E}(f_g(\omega)) \big] \big\|
$$

$$
(5.3.6) \qquad = \frac{1}{|G|} \sum_{g \in G} \sum_{\omega \in \Omega} \big\| R_{g^{-1}} \big[\mathrm{E}(f_g(\omega)) \big] \big\|
$$

$$
(5.3.7) \qquad = \frac{1}{|G|} \sum_{g \in G} \sum_{\omega \in \Omega} \big\| \mathrm{E}(f_g(\omega)) \big\|
$$

$$
(5.3.8) \qquad = \frac{1}{|G|} \sum_{g \in G} \sum_{\omega \in \Omega} \big\| \mathrm{E}(f_g(\omega)) \big\|
$$

$$
(5.3.9) \qquad \leq \|\mathrm{E}\|,
$$

where 5.3.7 follows from Wigner's theorem, and noting that (anti-)unitaries are norm preserving. ∎

Lemma 5.2. *The invariant mean of an observable is an observable.*

Proof. For any observable $\mathbf{E} : \Omega \to \mathscr{L}_s^+(\mathscr{H})$ the map $M_{R,f}(\mathbf{E})$ takes positive values since the R_g are positive, and the positive operators are a convex set. Further, if $\mathbf{E}$ is an observable then so is $M_{R,f}(\mathbf{E})$, since

$$(5.3.10) \qquad \sum_{\omega \in \Omega} M_{R,f}(\mathbf{E})(\omega) = \frac{1}{|G|} \sum_{\omega \in \Omega} \sum_{g \in G} R_{g^{-1}} \big[\mathbf{E}(f_g(\omega)) \big]$$

$$(5.3.11) \qquad = \frac{1}{|G|} \sum_{g \in G} R_{g^{-1}} \left[\sum_{\omega \in \Omega} \mathbf{E}(f_g(\omega)) \right]$$

$$(5.3.12) \qquad = \frac{1}{|G|} \sum_{g \in G} \mathrm{I}$$

$$(5.3.13) \qquad = \mathrm{I}.$$

$\blacksquare$

Lemma 5.3. *The invariant mean is the projection from $\mathscr{M}$ onto the subspace of (G, R, f)-covariant (in the sense of definition 2.4.2) maps.*

Proof. First note that $M_{R,f}$ is linear, since the R_g are linear. For any $\mathbf{E} \in \mathscr{M}$, $M_{R,f}(\mathbf{E})$ is covariant since

$$(5.3.14) \qquad M_{R,f}(\mathbf{E})(f_h(\omega)) = \frac{1}{|G|} \sum_{g \in G} R_{g^{-1}} \big[\mathbf{E}(f_g \circ f_h(\omega)) \big]$$

$$(5.3.15) \qquad = \frac{1}{|G|} \sum_{g' \in G} R_{(g'h^{-1})^{-1}} \big[\mathbf{E}(f_{g'h^{-1}} \circ f_h(\omega)) \big]$$

$$(5.3.16) \qquad = \frac{1}{|G|} \sum_{g' \in G} R_{hg'^{-1}} \big[\mathbf{E}(f_{g'}(\omega)) \big]$$

$$(5.3.17) \qquad = R_h \left[\frac{1}{|G|} \sum_{g' \in G} R_{g'^{-1}} \big[\mathbf{E}(f_{g'}(\omega)) \big] \right]$$

$$(5.3.18) \qquad = R_h \big[M_{R,f}(\mathbf{E})(\omega) \big].$$

Now (G, R, f)-covariant maps are invariant under $M_{R,f}$

$$(5.3.19) \qquad M_{R,f}(\mathbf{E})(\omega) = \frac{1}{|G|} \sum_{g \in G} R_{g^{-1}} \big[\mathbf{E}(f_g(\omega)) \big]$$

$$(5.3.20) \qquad = \frac{1}{|G|} \sum_{g \in G} R_{g^{-1}} \big[R_g [\mathbf{E}(\omega)] \big]$$

$$(5.3.21) \qquad = \frac{1}{|G|} \sum_{g \in G} \mathbf{E}(\omega)$$

$$(5.3.22) \qquad = \mathbf{E}(\omega),$$

so $M_{R,f}$ is idempotent. $\blacksquare$

It follows that the space of (G, R, f)-covariant maps is a vector subspace of $\mathcal{M}$, and that $\mathbf{E} = M_{R,f}(\mathbf{E})$ if, and only if, $\mathbf{E}$ is (G, R, f)-covariant.

Theorem 5.1. *Let G, $f_g : \Omega \to \Omega$ and $R_g : \mathscr{L}_s(\mathscr{H}) \to \mathscr{L}_s(\mathscr{H})$ satisfy the assumptions of definition 5.3.1. Let d be a jointly convex map from the probability distributions over Ω to $\mathbb{R}$, compatible with f_g in the sense that*

$$(5.3.23) \qquad\qquad d(P \circ f_g, Q \circ f_g) = d(P, Q),$$

for all probability distributions P, Q and all $g \in G$, then

$$(5.3.24) \qquad\qquad \sup_\rho d\left(M_{R,f}(\mathbf{E})^\rho, M_{R,f}(\mathbf{F})^\rho \right) \leq \sup_\rho d\left(\mathbf{E}^\rho, \mathbf{F}^\rho \right),$$

for all observables $\mathbf{E}, \mathbf{F} : \Omega \to \mathscr{L}_s^+(\mathscr{H})$.

Proof.

$$(5.3.25) \qquad \sup_\rho d\left(M_{R,f}(\mathbf{E})^\rho, M_{R,f}(\mathbf{F})^\rho \right) = \sup_\rho d\left(\frac{1}{|G|} \sum_{g \in G} \left(R_{g^{-1}} \circ \mathbf{E} \circ f_g \right)^\rho, \frac{1}{|G|} \sum_{g \in G} \left(R_{g^{-1}} \circ \mathbf{F} \circ f_g \right)^\rho \right)$$

$$(5.3.26) \qquad\qquad \leq \sup_\rho \frac{1}{|G|} \sum_{g \in G} d\left(\left(R_{g^{-1}} \circ \mathbf{E} \circ f_g \right)^\rho, \left(R_{g^{-1}} \circ \mathbf{F} \circ f_g \right)^\rho \right)$$

$$(5.3.27) \qquad\qquad \leq \frac{1}{|G|} \sum_{g \in G} \sup_\rho d\left(\left(R_{g^{-1}} \circ \mathbf{E} \circ f_g \right)^\rho, \left(R_{g^{-1}} \circ \mathbf{F} \circ f_g \right)^\rho \right)$$

$$(5.3.28) \qquad\qquad = \frac{1}{|G|} \sum_{g \in G} \sup_\rho d\left(\left(\mathbf{E} \circ f_g \right)^{R_{g^{-1}}^*[\rho]}, \left(\mathbf{F} \circ f_g \right)^{R_{g^{-1}}^*[\rho]} \right)$$

$$(5.3.29) \qquad\qquad \leq \frac{1}{|G|} \sum_{g \in G} \sup_\rho d\left(\left(\mathbf{E} \circ f_g \right)^\rho, \left(\mathbf{F} \circ f_g \right)^\rho \right)$$

$$(5.3.30) \qquad\qquad = \frac{1}{|G|} \sum_{g \in G} \sup_\rho d\left(\mathbf{E}^\rho \circ f_g, \mathbf{F}^\rho \circ f_g \right)$$

$$(5.3.31) \qquad\qquad = \frac{1}{|G|} \sum_{g \in G} \sup_\rho d\left(\mathbf{E}^\rho, \mathbf{F}^\rho \right)$$

$$(5.3.32) \qquad\qquad = \sup_\rho d\left(\mathbf{E}^\rho, \mathbf{F}^\rho \right).$$

∎

The compatibility condition (5.3.23) may arise for quite different reasons. The p-norm error measures defined in section 5.2 are invariant under all bijective functions on the outcome set[1], as are entropic quantities such as the Kullback-Leiber divergence. On the other hand the Wasserstein metrics mentioned in section 2.5 are only compatible with maps which leave the underlying metric on Ω invariant, for example where $\Omega = \mathbb{R}$ the standard metric on $\mathbb{R}$ is

---

[1]Elements of a group action must be invertible, and hence bijective.

compatible with translations. In the proof of theorem 5.1 we only require that $d(P \circ f_g, Q \circ f_g) \leq d(P, Q)$, however this being true for all $g \in G$ implies equality.

Given a set of $n \in \mathbb{N}$ finite sets $\{\Omega_i \,|\, i \in 1 \ldots n\}$, and n finite groups $\{G_i \,|\, i \in 1 \ldots n\}$, with action $f^i_{g_i} : \Omega_i \to \Omega_i$, for each $g_i \in G_i$ there is a *product action* π of the direct product group $G = \prod_i G_i$ on the Cartesian product set $\Omega = \prod_i \Omega_i$

$$(5.3.33) \qquad \pi_g : \Omega \to \Omega, \quad \forall g \in G$$

$$(5.3.34) \qquad \pi_{(g_1, \ldots, g_i, \ldots, g_n)} : (\omega_1, \ldots \omega_n) \mapsto (f^1_{g_1}(\omega_1), \ldots, f^n_{g_n}(\omega_n)),$$

there is also a marginal action μ^i of the direct product group on each Ω_i

$$(5.3.35) \qquad \mu^i_g : \Omega_i \to \Omega_i, \quad \forall g \in G$$

$$(5.3.36) \qquad \mu^i_{(g_1, \ldots, g_i, \ldots, g_n)} : \omega \mapsto f^i_{g_i}(\omega).$$

Lemma 5.4. *For $i \in 1 \ldots n$ let $\mathrm{E}_i : \Omega_i \to \mathscr{L}^+_s(\mathscr{H})$ be a compatible family of observables, and $\{G_i \,|\, i \in 1 \ldots n\}$ be a set of groups, such that G_i has action f^i_g on Ω_i. Let $\Omega = \prod_i \Omega_i$ be the Cartesian product, $G = \prod_i G_i$ the direct product, and π, μ^i the product and marginal actions of G respectively. Let $\{R_g \,|\, g \in G\}$ be a representation of G as positive, unital, linear maps acting on $\mathscr{L}_s(\mathscr{H})$. If J is any Cartesian joint observable for the E_i, and $\tilde{\mathrm{J}}_i$ the ith margin of $M_{R,\pi}(\mathrm{J})$,*

$$(5.3.37) \qquad \tilde{\mathrm{J}}_i : \Omega_i \to \mathscr{L}^+_s(\mathscr{H})$$

$$(5.3.38) \qquad \tilde{\mathrm{J}}_i : \omega^* \mapsto \sum_{\substack{\boldsymbol{\omega} \in \Omega \\ \omega_i = \omega^*}} M_{R,\pi}(\mathrm{J})(\boldsymbol{\omega}),$$

where ω_i denotes the ith element of the tuple $\boldsymbol{\omega}$, then

$$(5.3.39) \qquad \tilde{\mathrm{J}}_i(\omega) = M_{R,\mu^i}(\mathrm{E}_i)(\omega), \quad \forall \omega \in \Omega_i.$$

Proof.

$$\tilde{\mathbf{J}}_i(\omega^*) = \sum_{\substack{\boldsymbol{\omega}\in\Omega \\ \omega_i=\omega^*}} M_{R,\pi}(\mathbf{J})(\boldsymbol{\omega}) \tag{5.3.40}$$

$$= \sum_{\substack{\boldsymbol{\omega}\in\Omega \\ \omega_i=\omega^*}} \frac{1}{|G|}\sum_{g\in G} R_{g^{-1}}\left[\mathbf{J}(\pi_g(\boldsymbol{\omega}))\right] \tag{5.3.41}$$

$$= \frac{1}{|G|}\sum_{g\in G} R_{g^{-1}}\left[\sum_{\substack{\boldsymbol{\omega}\in\Omega \\ \omega_i=\omega^*}} \mathbf{J}(\pi_g(\boldsymbol{\omega}))\right] \tag{5.3.42}$$

$$= \frac{1}{|G|}\sum_{g\in G} R_{g^{-1}}\left[\sum_{\substack{\boldsymbol{\omega}\in\Omega \\ \pi_{g^{-1}}(\boldsymbol{\omega})_i=\omega^*}} \mathbf{J}(\boldsymbol{\omega})\right] \tag{5.3.43}$$

$$= \frac{1}{|G|}\sum_{g\in G} R_{g^{-1}}\left[\sum_{\substack{\boldsymbol{\omega}\in\Omega \\ \omega_i=\mu_g^i(\omega^*)}} \mathbf{J}(\boldsymbol{\omega})\right] \tag{5.3.44}$$

$$= \frac{1}{|G|}\sum_{g\in G} R_{g^{-1}}\left[\mathbf{E}\left(\mu_g^i(\omega^*)\right)\right] \tag{5.3.45}$$

$$= M_{R,\mu^i}(\mathbf{E}_i)(\omega^*). \tag{5.3.46}$$

∎

Theorem 5.2. *Let* $\{\mathbf{E}_i\,|\,i\in 1\dots n\}$ *be a family of (not necessarily compatible) observables,* $\mathbf{E}_i: \Omega_i \to \mathscr{L}_s^+(\mathscr{H})$, *and* $\{G_i\,|\,i\in 1\dots n\}$ *be a set of groups, such that* G_i *has action* f_g^i *on* Ω_i. *Let* $\Omega = \prod_i \Omega_i$ *be the Cartesian product,* $G = \prod_i G_i$ *the direct product, and* π, μ^i *the product and marginal actions of* G *respectively. Let* $\{R_g\,|\,g\in G\}$ *be a representation of* G *as positive, unital, linear maps acting on* $\mathscr{L}_s(\mathscr{H})$ *such that*

$$M_{R,\mu^i}(\mathbf{E}_i) = \mathbf{E}_i. \tag{5.3.47}$$

Then for any compatible family of observables $\{\mathbf{F}_i\,|\,i\in 1\dots n\}$, $\mathbf{F}_i: \Omega_i \to \mathscr{L}_s^+(\mathscr{H})$, *with joint observable* $\mathbf{J}: \Omega \to \mathscr{L}_s^+(\mathscr{H})$, *the observables*

$$\tilde{\mathbf{F}}_i = M_{R,\mu^i}(\mathbf{F}_i) \tag{5.3.48}$$

are compatible, with joint $\tilde{\mathbf{J}} = M_{R,\pi}(\mathbf{J})$, *and for any function* d *satisfying the constraints of theorem 5.1*

$$\sup_\rho d(\tilde{\mathbf{F}}_i^\rho, \mathbf{E}_i^\rho) \le \sup_\rho d(\mathbf{F}_i^\rho, \mathbf{E}_i^\rho). \tag{5.3.49}$$

Proof. The compatibility of the $\tilde{\mathbf{F}}_i$ follows directly from lemma 5.4, it only remains to establish inequality (5.3.49),

$$(5.3.50) \qquad \sup_\rho d(\tilde{\mathbf{F}}_i, \mathbf{E}_i) = \sup_\rho d(M_{R,\mu^i}(\mathbf{F}), \mathbf{E}_i)$$

$$(5.3.51) \qquad = \sup_\rho d(M_{R,\mu^i}(\mathbf{F}), M_{R,\mu^i}(\mathbf{E}_i))$$

$$(5.3.52) \qquad \leq d(\mathbf{F}_i, \mathbf{E}_i).$$

where (5.3.51) is a consequence of assuming the target observables are unchanged by the invariant mean, and (5.3.52) is the result of theorem 5.1. ∎

It is tempting to attempt to generalise equation (5.3.2), and, for a locally compact group G, with (left) Haar measure μ, continuous action $\alpha : (g, \omega) \mapsto g \cdot \omega$ on a Borel measurable, locally compact space $(\Omega, \mathscr{F})$, and continuous representation R_g, on $\mathscr{L}_s^+(\mathscr{H})$ define

$$(5.3.53) \qquad M[F] : X \mapsto \int_G d\mu(g) R_g[F(g.X)],$$

for a POVM $F : \mathscr{F} \to \mathscr{L}_s^+(\mathscr{H})$. Unfortunately there are significant technical obstacles to defining such a quantity. In particular one would have to show the function $g \mapsto R_g[F(g.X)]$ is μ-measurable, in the sense of the Bochner integral [24], either for all observables, or for a physically relevant subset. In the (possibly highly restricted) cases that such a quantity may be defined it is easy to see that it will be necessary for the group G to be compact, rather than locally compact since

$$(5.3.54) \qquad M[F] : \Omega \mapsto \int_G d\mu(g) R_g[F(g.\Omega)]$$

$$(5.3.55) \qquad = \int_G d\mu(g) R_g[\mathrm{I}]$$

$$(5.3.56) \qquad = \mathrm{I} \int_G d\mu(g).$$

The Haar measure μ may be normalised to a probability measure if, and only if, the group is compact. This excludes several physically relevant groups including the translation group of $\mathbb{R}$ or $\mathbb{R}^n$, the Galilei group and the Poincaré group. Compact groups relevant to physical applications include the finite groups covered above, the unitary, special unitary groups, orthogonal and special orthogonal groups in $n \in \mathbb{N}$ dimensions.

The generalised invariant mean will require additional regularity conditions on the observables it is applied to. To see why this is the case we recall that to be Bochner integrable the function $g \mapsto R_g[F(g.X)]$ must be the limit of piecewise constant functions, where the pieces are measurable sets. To take a concrete example we restrict our attention to probability measures on the circle. Let $\Omega = [-\pi, \pi)$, (Ω, τ) be the topological space of the unit circle, $X = (0, 1) \subset \Omega$, $F : \mathscr{B}(\Omega, \tau) \to [0, 1]$ be the point measure, assigning 1 to sets if they contain the element 0, and 0 otherwise otherwise, finally take G to be the circle group and $f_g : h \mapsto gh$ be the action of the

circle group on itself. Consider a sequence g_n of negative elements of Ω, converging to zero, then

$$(5.3.57) \qquad F(f_{g_n}(X)) = F(g_n + X)$$

$$(5.3.58) \qquad = F((g_n, 1 + g_n))$$

$$(5.3.59) \qquad = 1,$$

whereas $F(X) = 0$. With general observables it is difficult to control these discontinuities. We conjecture that a necessary and sufficient condition for measurability is the existence of a covariant observable dominating F.

5.4 Increasing the error

Applying the techniques in section 5.3 results leads to compatible approximations that are "not worse than" any other compatible approximations, in the sense that for any family of compatible approximations to the targets, there exists a covariant family of compatible approximations with d_p values less than or equal to the original family. It is therefore useful to know when we can *increase* the d_p values so we can cover the entire uncertainty region with convex combinations of covariant and trivial observables.

Lemma 5.5 (Increasing the error - ∞-norm)**.** *Let* $\{\mathbf{E}_i\}$ *be a family of observables with outcome sets* Ω_i*. Choose* $i \in 1 \ldots n$ *and* $\boldsymbol{v} = (v_1 \ldots v_i \ldots v_n) \in S_\infty(\mathbf{E}_1 \ldots \mathbf{E}_n)$*, such that there exists some* $\omega^* \in \Omega_i$ *where* $\mathbf{E}_i(\omega^*)$ *is not of full rank, then* $v_i \leq v_i' \leq 1 \implies \boldsymbol{v}' = (v_1 \ldots v_i' \ldots v_n) \in S_\infty(\mathbf{E}_1 \ldots \mathbf{E}_n)$*.*

Proof. Let $\Omega = \prod_i \Omega_i$ be the Cartesian product of the outcome sets, since $\boldsymbol{v} \in S_\infty(\mathbf{E}_1 \ldots \mathbf{E}_n)$ there exists a compatible family of observables $\mathbf{F}_i$ with joint $\mathbf{J} : \Omega \to \mathscr{L}_s(\mathscr{H})$ such that

$$(5.4.1) \qquad d_\infty(\mathbf{E}_i, \mathbf{F}_i) = v_i$$

Now define

$$(5.4.2) \qquad \tilde{\mathbf{J}} : \Omega \to \mathscr{L}_s(\mathscr{H})$$

$$(5.4.3) \qquad \tilde{\mathbf{J}} : (\omega_1 \ldots \omega_n) \mapsto \begin{cases} \sum_{\omega \in \Omega_i} \mathbf{J}(\omega_1 \ldots \omega_{i-1}, \omega, \omega_{i+1} \ldots \omega_n), & \omega_i = \omega^* \\ 0, & \text{else} \end{cases},$$

Let $\tilde{\mathbf{F}}_j$ be the jth Cartesian margin of $\tilde{\mathbf{J}}$, and note that for $j \neq i$ we have $\tilde{\mathbf{F}}_j = \mathbf{F}_j$, but that $\tilde{\mathbf{F}}_i : \omega \mapsto \delta_{\omega \omega^*} \mathbf{I}$ is the trivial observable which gives outcome ω^* with certainty in any state. Since $\mathbf{E}_i(\omega^*)$ is not of full rank, there exists a pure state ρ such that $\text{tr}\left(\mathbf{E}_i(\omega^*)\rho\right) = 0$; therefore $d_\infty(\mathbf{E}_i, \tilde{\mathbf{F}}_i) = 1$.

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We can now define the observable $\mathbf{J}_\lambda = (1-\lambda)\mathbf{J} + \lambda\tilde{\mathbf{J}}$, for $\lambda \in [0,1]$, with margins $\mathbf{F}_{j\lambda}$. As before we have $j \neq i \implies \mathbf{F}_{j\lambda} = \mathbf{F}_j$, but $\mathbf{F}_{i,\lambda} = (1-\lambda)\mathbf{F}_i + \lambda\tilde{\mathbf{F}}_i$. We can compute the distance

$$(5.4.4) \qquad d_\infty(\mathbf{E}_i, \mathbf{F}_{i\lambda}) = \sup_{\rho \in \mathscr{S}(\mathscr{H})} \max_{\omega \in \Omega} \left| \operatorname{tr}\left(\rho(\mathbf{E}_i(\omega) - \mathbf{F}_{i\lambda}(\omega))\right) \right|$$

$$(5.4.5) \qquad = \sup_{\rho \in \mathscr{S}(\mathscr{H})} \max_{\omega \in \Omega} \left| (1-\lambda)\operatorname{tr}\left(\rho(\mathbf{E}_i(\omega) - \mathbf{F}_i)\right) + \lambda \operatorname{tr}\left(\rho(\mathbf{E}_i(\omega) - \tilde{\mathbf{F}}_i)\right)(\omega) \right|,$$

as we take the $\sup_\rho$ over a compact set, so $\lambda \mapsto d_\infty(\mathbf{E}_i, \mathbf{F}_{i\lambda})$ is a continuous function from $[0,1] \to \mathbb{R}^+$, by the intermediate value theorem every value between $d_\infty(\mathbf{E}_i, \mathbf{F}_i)$ and $d_\infty(\mathbf{E}_i, \tilde{\mathbf{F}}_i) = 1$ is achieved by some λ. ∎

Lemma 5.6 (Increasing the error - p-norm)**.** *Let $\{\mathbf{E}_i\}$ be a family of observables with outcome sets Ω_i. Choose $i \in 1 \ldots n$ and $\boldsymbol{v} = (v_1 \ldots v_i \ldots v_n) \in S_p(\mathbf{E}_1 \ldots \mathbf{E}_n)$, such that there exists some $\omega^* \in \Omega_i$ where $\operatorname{tr}\left(\mathbf{E}_i(\omega^*)\rho^*\right) = 1$ for some $\rho^* \in \mathscr{S}(\mathscr{H})$ then $v_i \leq v_i' \leq 2^{\frac{1}{p}} \implies \boldsymbol{v}' = (v_1 \ldots v_i' \ldots v_n) \in S_p(\mathbf{E}_1 \ldots \mathbf{E}_n)$.*

Proof. Let $\Omega = \prod_i \Omega_i$ be the Cartesian product of the outcome sets, since $\boldsymbol{v} \in S_p(\mathbf{E}_1 \ldots \mathbf{E}_n)$ there exists a compatible family of observables $\mathbf{F}_i$ with joint $\mathbf{J} : \Omega \to \mathscr{L}_s(\mathscr{H})$ such that

$$(5.4.6) \qquad d_p(\mathbf{E}_i, \mathbf{F}_i) = v_i$$

Now choose $\tilde{\omega} \neq \omega^*$ and define

$$(5.4.7) \qquad \tilde{\mathbf{J}} : \Omega \to \mathscr{L}_s(\mathscr{H})$$

$$(5.4.8) \qquad \tilde{\mathbf{J}} : (\omega_1 \ldots \omega_n) \mapsto \begin{cases} \sum_{\omega \in \Omega_i} \mathbf{J}(\omega_1 \ldots \omega_{i-1}, \omega, \omega_{i+1} \ldots \omega_n), & \omega_i = \tilde{\omega} \\ 0, & \text{else} \end{cases},$$

Let $\tilde{\mathbf{F}}_j$ be the jth Cartesian margin of $\tilde{\mathbf{J}}$, and note that for $j \neq i$ we have $\tilde{\mathbf{F}}_j = \mathbf{F}_j$, but that $\tilde{\mathbf{F}}_i : \omega \mapsto \delta_{\omega\tilde{\omega}}\mathbf{I}$ is the trivial observable which gives outcome $\tilde{\omega}$ with certainty in any state. Since we have $\operatorname{tr}\left(\mathbf{E}(\omega^*)\rho^*\right) = 1$ we can compute

$$(5.4.9) \qquad d_p(\mathbf{E}_i, \tilde{\mathbf{F}}_i) = \sup_\rho \left(\sum_{\omega \in \Omega_i} \left| \operatorname{tr}\left(\rho(\mathbf{E}_i(\omega) - \tilde{\mathbf{F}}_i(\omega))\right) \right|^p \right)^{\frac{1}{p}}$$

$$(5.4.10) \qquad \geq \left(\sum_{\omega \in \Omega_i} \left| \operatorname{tr}\left(\rho^*(\mathbf{E}_i(\omega) - \tilde{\mathbf{F}}_i(\omega))\right) \right|^p \right)^{\frac{1}{p}}$$

$$(5.4.11) \qquad = \left(\left| \operatorname{tr}\left(\rho^*\tilde{\mathbf{F}}_i(\tilde{\omega})\right) \right|^p + \left| \operatorname{tr}\left(\rho^*\mathbf{E}_i(\omega^*)\right) \right|^p \right)^{\frac{1}{p}}$$

$$(5.4.12) \qquad = 2^{\frac{1}{p}}$$

We can now define the observable $\mathbf{J}_\lambda = (1-\lambda)\mathbf{J} + \lambda\tilde{\mathbf{J}}$, for $\lambda \in [0,1]$, with margins $F_{j\lambda}$. As before we have $j \neq i \implies \mathbf{F}_{j\lambda} = \mathbf{F}_j$, but $\mathbf{F}_{i,\lambda} = (1-\lambda)\mathbf{F}_i + \lambda\tilde{\mathbf{F}}_i$. We can compute the distance

$$(5.4.13) \qquad d_p(\mathbf{E}_i, \mathbf{F}_{i,\lambda}) = \sup_\rho \left(\sum_{\omega \in \Omega_i} \left| \operatorname{tr}\left(\rho(\mathbf{E}_i(\omega) - \tilde{\mathbf{F}}_{i\lambda}(\omega))\right) \right|^p \right)^{\frac{1}{p}},$$

as we take the $\sup_\rho$ over a compact set, $\lambda \mapsto d(\mathrm{E}_i, \mathrm{F}_{i,\lambda})$ is a continuous function from $[0,1] \to \mathbb{R}^+$. By the intermediate value theorem every value between $d(\mathrm{E}_i, \mathrm{F}_i)$ and $d(\mathrm{E}_i, \tilde{\mathrm{F}}_i) = 2^{\frac{1}{p}}$ is achieved by some λ. ∎

5.5 The qubit triple

Let $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ be three orthonormal vectors in $\mathbb{R}^3$, and consider the three, two-outcome qubit observables

$$(5.5.1) \qquad \mathrm{A}: \{+1,-1\} \to \mathscr{L}\left(\mathbb{C}^2\right), \qquad \mathrm{B}: \{+1,-1\} \to \mathscr{L}\left(\mathbb{C}^2\right), \qquad \mathrm{C}: \{+1,-1\} \to \mathscr{L}\left(\mathbb{C}^2\right)$$

$$(5.5.2) \qquad \mathrm{A}: k \mapsto \frac{1}{2}(\mathrm{I} + k\boldsymbol{a}\cdot\boldsymbol{\sigma}), \qquad \mathrm{B}: l \mapsto \frac{1}{2}(\mathrm{I} + l\boldsymbol{b}\cdot\boldsymbol{\sigma}), \qquad \mathrm{C}: m \mapsto \frac{1}{2}(\mathrm{I} + m\boldsymbol{c}\cdot\boldsymbol{\sigma}).$$

We would like to find the set

$$(5.5.3)$$
$$S(\mathrm{A},\mathrm{B},\mathrm{C}) = \left\{ (d(\mathrm{A},\mathrm{D}), d(\mathrm{B},\mathrm{E}), d(\mathrm{C},\mathrm{F})) \,\middle|\, \mathrm{D},\mathrm{E},\mathrm{F}: \{+1,-1\} \to \mathscr{L}\left(\mathbb{C}^2\right) \text{ are compatible} \right\} \subseteq [0,1]^3.$$

The condition D, E, F are compatible is equivalent to the existence of an observable $\mathrm{J}: \{+1,-1\}^3 \to \mathscr{L}\left(\mathbb{C}^2\right)$ such that

$$(5.5.4) \qquad \sum_{l,m} \mathrm{J}(k,l,m) = \mathrm{D}(k)$$

$$(5.5.5) \qquad \sum_{k,m} \mathrm{J}(k,l,m) = \mathrm{E}(l)$$

$$(5.5.6) \qquad \sum_{k,l} \mathrm{J}(k,l,m) = \mathrm{F}(m).$$

Since we have three, two-outcome target observables we take as our product group the elementary Abelian group of order 8, the additive group of the vector space $(\mathbb{Z}/2\mathbb{Z})^3$

$$(5.5.7) \qquad G = \left\{ g(k,l,m) \,\middle|\, (k,l,m) \in \{+1,-1\}^3 \right\}$$

$$(5.5.8) \qquad g(h,i,j)g(k,l,m) = g(hk,il,jm),$$

this group has product action on the outcome set $\{+1,-1\}^3$

$$(5.5.9) \qquad \pi_{h,i,j}((k,l,m)) = (hk,il,jm),$$

and marginal actions

$$(5.5.10) \qquad \mu^1_{h,i,j}(k) = hk$$

$$(5.5.11) \qquad \mu^2_{h,i,j}(l) = il$$

$$(5.5.12) \qquad \mu^3_{h,i,j}(m) = jm$$

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and may be represented by the following set of positive, unital, linear maps on $\mathscr{L}_s(\mathbb{C}^2)$

$$(5.5.13) \qquad R_{k,l,m}\left[\frac{1}{2}\left(r_0\,\mathrm{I}+\begin{pmatrix}r_1\\r_2\\r_3\end{pmatrix}\cdot\boldsymbol{\sigma}\right)\right]=\frac{1}{2}\left(r_0\,\mathrm{I}+\begin{pmatrix}kr_1\\lr_2\\mr_3\end{pmatrix}\cdot\boldsymbol{\sigma}\right).$$

Given any compatible two-outcome qubit observables, $\mathbf{D}$, $\mathbf{E}$ and $\mathbf{F}$, we can apply the invariant mean with respect to this group, action and representation to the joint $\mathbf{J}$

$$(5.5.14) \qquad \tilde{\mathbf{J}}(k,l,m)=\frac{1}{8}\sum_{(h,i,j)\in\{+1,-1\}^3}R_{h,i,j}[\mathbf{J}(hk,il,jm)],$$

and take the margins of the $\tilde{\mathbf{J}}$ to get a new set of compatible, two outcome qubit observables

$$(5.5.15) \qquad \tilde{\mathbf{D}}(k)=\sum_{(l,m)\in\{+1,-1\}^2}\tilde{\mathbf{J}}(k,l,m)$$

$$(5.5.16) \qquad \tilde{\mathbf{E}}(l)=\sum_{(k,m)\in\{+1,-1\}^2}\tilde{\mathbf{J}}(k,l,m)$$

$$(5.5.17) \qquad \tilde{\mathbf{F}}(m)=\sum_{(k,l)\in\{+1,-1\}^2}\tilde{\mathbf{J}}(k,l,m).$$

By lemma 5.4 this is equivalent to taking the invariant mean with respect to the G, R and μ^i of $\mathbf{D}$, $\mathbf{E}$, $\mathbf{F}$ directly

$$(5.5.18) \qquad \tilde{\mathbf{D}}(k)=M_{R,f^1}(\mathbf{D})(k)\qquad\tilde{\mathbf{E}}(l)=M_{R,f^2}(\mathbf{E})(l)\qquad\tilde{\mathbf{F}}(m)=M_{R,f^3}(\mathbf{F})(m)$$

These margin groups, actions and representations satisfy all of the requirements of lemma 5.2 above, so the group averaging maps reduce the error. We also have that $M_{R,\mu^1}(\mathbf{A})=\mathbf{A}$ etc. so we can apply theorem 5.2 implying that for every compatible triple $\mathbf{D}$, $\mathbf{E}$, $\mathbf{F}$ there exists a *covariant* compatible triple with lower distances to the targets. Since we can also increase the distances using lemma 5.5 as needed we can fill the set $S(\mathbf{A},\mathbf{B},\mathbf{C})$ by searching over the covariant observables, and then increasing the distances up to the trivial maximum of $2^{\frac{1}{p}}$. The covariant joints have the form

$$(5.5.19) \qquad \mathbf{J}(k,l,m)=\frac{1}{8}\left(\mathrm{I}+\begin{pmatrix}kj_1\\lj_2\\mj_3\end{pmatrix}\cdot\boldsymbol{\sigma}\right),$$

for $\|\boldsymbol{j}\|\leq 1$. The margins have the form

$$(5.5.20) \qquad \mathbf{D}(k)=\frac{1}{2}(\mathrm{I}+kj_1\boldsymbol{a}\cdot\boldsymbol{\sigma})\qquad \mathbf{E}(l)=\frac{1}{2}(\mathrm{I}+lj_2\boldsymbol{b}\cdot\boldsymbol{\sigma})\qquad \mathbf{F}(m)=\frac{1}{2}(\mathrm{I}+mj_3\boldsymbol{c}\cdot\boldsymbol{\sigma}),$$

which have distances

$$(5.5.21) \qquad d_p(\mathbf{A},\mathbf{D})=2^{\frac{1}{p}-1}(1-j_1)\qquad d_p(\mathbf{B},\mathbf{E})=2^{\frac{1}{p}-1}(1-j_2)\qquad d_p(\mathbf{C},\mathbf{F})=2^{\frac{1}{p}-1}(1-j_3).$$

Hence the positivity constraint $\|\boldsymbol{j}\| \leq 1$ becomes

$$(5.5.22) \qquad \left(d(\mathrm{A},\mathrm{D})-2^{\frac{1}{p}-1}\right)^2 + \left(d(\mathrm{B},\mathrm{E})-2^{\frac{1}{p}-1}\right)^2 + \left(d(\mathrm{C},\mathrm{F})-2^{\frac{1}{p}-1}\right)^2 \leq 2^{\frac{2}{p}-2}.$$

The subset of S_p covered by covariant observables is a sphere of radius $2^{\frac{1}{p}-1}$ centered at $\left(2^{\frac{1}{p}-1}, 2^{\frac{1}{p}-1}, 2^{\frac{1}{p}-1}\right)$, the full region is the monotone closure of this within the cube $[0, 2^{\frac{1}{p}}]^3$ and is plotted in figure 5.2. We compare this to the work of Busch and Heinosaari [12] and Heinosaari, Stano and Reitzner [40], the authors consider measurement uncertainty regions for pairs of sharp, two-outcome qubit observables with a measure of statistical distance that is equivalent to ours (identical up to a multiplicative constant). They determine semi-analytical bounds for arbitrary pairs of such observables and tight, analytical bounds for the case where the two observables are mututually unbiased (i.e. the Bloch vectors are orthogonal). This latter case is contained as a two-dimensional slice through the uncertainty region for three observables which we have determined in this section. More precisely the uncertainty region determined in those papers is the slice through the region plotted in figure 5.2 where $d_\infty(\mathrm{C},\mathrm{F}) = 1$.

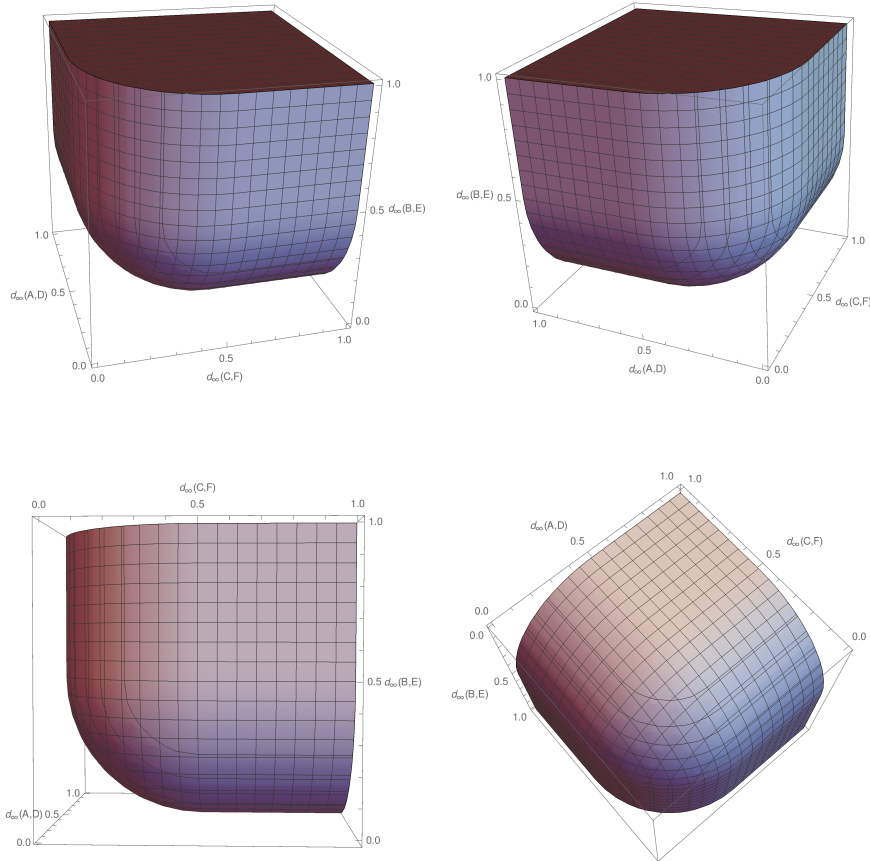

Figure 5.2: Various views of the uncertainty region for three mutually unbiased qubit observables $S_\infty(\mathrm{A},\mathrm{B},\mathrm{C})$ covered by compatible approximations D, E and F.

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5.6   The Fourier pair

Let $\mathbb{Z}_n = \{0 \dots n-1\}$ denote the cyclic group of order n, equivalent to the set of natural numbers less than n, with the group operation addition modulo n, denoted $+$. Although this is only a field for n prime, it will be useful to define multiplication, denoted by juxtaposition, as the usual multiplication of natural numbers modulo n.

Let $\mathcal{H}$ be a Hilbert space of dimension $n \in \mathbb{N}$, $n \geq 2$, $\{|g\rangle \,|\, g \in \mathbb{Z}_n\}$ be an orthonormal set of vectors, hereafter called the *computational basis* and let

$$(5.6.1) \qquad |f_h\rangle := \sqrt{\frac{1}{n}} \sum_{g \in \mathbb{Z}_n} e^{\frac{2\pi i}{n} gh} |g\rangle, \quad h \in \mathbb{Z}_n$$

$$(5.6.2) \qquad \implies |g\rangle = \sqrt{\frac{1}{n}} \sum_{h \in \mathbb{Z}_n} e^{-\frac{2\pi i}{n} gh} |f_h\rangle, \quad g \in \mathbb{Z}_n$$

be the well known *Fourier basis*. It is easily verified that the $|f_h\rangle$ are an orthonormal basis for $\mathcal{H}$ and are *mutually unbiased* with the computational basis. We define sharp observables for these bases

$$(5.6.3) \qquad \mathrm{A} : \mathbb{Z}_n \to \mathscr{L}_s^+(\mathcal{H}) \qquad\qquad \mathrm{B} : \mathbb{Z}_n \to \mathscr{L}_s^+(\mathcal{H})$$

$$(5.6.4) \qquad \mathrm{A} : g \mapsto |g\rangle\langle g| \qquad\qquad \mathrm{B} : h \mapsto |f_h\rangle\langle f_h|.$$

We can define unitary *shift operators* for these bases

$$(5.6.5) \qquad U_k |g\rangle = |g+k\rangle \qquad\qquad \forall g, k \in \mathbb{Z}_n$$

$$(5.6.6) \qquad V_q |f_h\rangle = |f_{h+q}\rangle \qquad\qquad \forall h, q \in \mathbb{Z}_n,$$

and note that each form a unitary representation of the group $\mathbb{Z}_n$. Further, we have that

$$(5.6.7) \qquad U_k = \sum_{h \in \mathbb{Z}_n} e^{-\frac{2\pi i}{n} kh} |f_h\rangle\langle f_h| = \sum_{h \in \mathbb{Z}_n} e^{-\frac{2\pi i}{n} kh} \,\mathrm{B}(h)$$

$$(5.6.8) \qquad V_q = \sum_{g \in \mathbb{Z}_n} e^{\frac{2\pi i}{n} qg} |g\rangle\langle g| = \sum_{g \in \mathbb{Z}_n} e^{\frac{2\pi i}{n} qg} \,\mathrm{A}(g).$$

It is easy to verify the commutation relations

$$(5.6.9) \qquad U_k V_q = e^{\frac{2\pi i}{n} kq} V_q U_k,$$

by, for example, applying the operator on each side of the equality to the states in the Fourier basis. These are exactly the Weyl commutation relations for the discrete Heisenberg (or Heisenberg-Weyl) group [36]. It follows that

$$(5.6.10) \qquad U_k V_q \rho V_q^\dagger U_k^\dagger = V_q U_k \rho U_k^\dagger V_q^\dagger, \quad \forall \rho \in \mathscr{L}_s(\mathcal{H}), k, q \in \mathbb{Z}_n.$$

We therefore consider the linear maps

$$(5.6.11) \qquad R_{k,q} : \mathscr{L}_s(\mathscr{H}) \to \mathscr{L}_s(\mathscr{H})$$

$$(5.6.12) \qquad R_{k,q} : \rho \mapsto U_k V_q \rho V_q^\dagger U_k^\dagger = V_q U_k \rho U_k^\dagger V_q^\dagger,$$

and note that they form a representation of the direct product group $G = \mathbb{Z}_n \times \mathbb{Z}_n$, with the group operation given by operator composition

$$(5.6.13) \qquad R_{k,q} \circ R_{l,r} = R_{k+l,p+r}, \quad \forall k,l,q,r \in \mathbb{Z}_n.$$

These maps act on the effects of the target observables correctly

$$(5.6.14) \qquad R_{k,q}[|g\rangle\langle g|] = |g+k\rangle\langle g+k|$$

$$(5.6.15) \qquad R_{k,q}[|f_h\rangle\langle f_h|] = |f_{h+q}\rangle\langle f_{h+q}|.$$

Therefore we can apply the theorems of section 5.3 to establish that the covariant joint observables are optimal with respect to the d_p distance measures.

5.6.1 Commutivity

There is a one-to-one relation between covariant joint observables $\mathsf{J} : \mathbb{Z}_n \times \mathbb{Z}_n \to \mathscr{L}_s^+(\mathscr{H})$ and trace one positive operators on $\mathscr{H}$ given by

$$(5.6.16) \qquad \mathsf{J} : (k,q) \mapsto \frac{1}{n} R_{k,q}[\tau].$$

All covariant, $\mathbb{Z}_n \times \mathbb{Z}_n$ valued observable are obtained in this way, for some trace 1 positive τ, as we can take $\tau = n\mathsf{J}(0,0)$, and all trace 1 positive operators give rise to some covariant, $\mathbb{Z}_n \times \mathbb{Z}_n$ valued observable. We can write down the margins of such an observable

$$(5.6.17) \qquad \mathsf{C} : \mathbb{Z}_n \to \mathscr{L}_s^+(\mathscr{H}) \qquad\qquad \mathsf{D} : \mathbb{Z}_n \to \mathscr{L}_s^+(\mathscr{H})$$

$$(5.6.18) \qquad \mathsf{C} : g \mapsto \sum_h \mathsf{J}(g,h) = \frac{1}{n}\sum_h R_{g,h}[\tau] \qquad \mathsf{D} : h \mapsto \sum_g \mathsf{J}(g,h) = \frac{1}{n}\sum_g R_{g,h}[\tau].$$

We can show that each $\mathsf{C}(k)$ commutes with each V_q

$$(5.6.19) \qquad \mathsf{C}(g) = \sum_h \mathsf{J}(g,h)$$

$$(5.6.20) \qquad = \sum_h \mathsf{J}(g,h+q)$$

$$(5.6.21) \qquad = \sum_h R_{0,q}[\mathsf{J}(g,h)]$$

$$(5.6.22) \qquad = V_q \mathsf{C}(g) V_q^*$$

$$(5.6.23) \qquad \implies \mathsf{C}(g) V_q = V_q \mathsf{C}(g), \quad \forall g,q \in \mathbb{Z}_n.$$

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A similar calculation gives

$$(5.6.24) \qquad D(h)U_k = U_k D(h), \quad \forall h, k \in \mathbb{Z}_n.$$

Indeed an explicit calculation gives

$$(5.6.25) \qquad C(g) = \sum_k |k+g\rangle\langle k+g| \langle k|\tau|k\rangle$$

$$(5.6.26) \qquad D(h) = \sum_q |f_{q+h}\rangle\langle f_{q+h}| \langle f_q|\tau|f_q\rangle.$$

5.6.2 Computing the sup-norm

The simultaneous diagonalisability of A and C allows us to compute $d_\infty(A, C)$ explicitly. Without loss of generality let

$$(5.6.27) \qquad C(0) = \sum_{k \in \mathbb{Z}_n} c_k |k\rangle\langle k|$$

for $c_k \in [0, 1]$, and $\sum_k c_k = 1$. Then

$$(5.6.28) \qquad d_\infty(A, C) = \sup_\rho \max_g \left| \mathrm{tr}\left(\rho[A(g) - C(g)] \right) \right|$$

$$(5.6.29) \qquad = \sup_\rho \max_g \left| \mathrm{tr}\left(\rho \left[|g\rangle\langle g| - U_g \sum_{k \in \mathbb{Z}_n} c_k |k\rangle\langle k| U_g^\dagger \right] \right) \right|$$

$$(5.6.30) \qquad = \sup_\rho \max_g \left| \mathrm{tr}\left(\rho U_g \left[|0\rangle\langle 0| - \sum_{k \in \mathbb{Z}_n} c_k |k\rangle\langle k| \right] U_g^\dagger \right) \right|$$

$$(5.6.31) \qquad = \sup_\rho \max_g \left| \mathrm{tr}\left(U_g^\dagger \rho U_g \left[|0\rangle\langle 0| - \sum_{k \in \mathbb{Z}_n} c_k |k\rangle\langle k| \right] \right) \right|$$

$$(5.6.32) \qquad = \sup_\rho \left| \mathrm{tr}\left(\rho \left[|0\rangle\langle 0| - \sum_{k \in \mathbb{Z}_n} c_k |k\rangle\langle k| \right] \right) \right|$$

$$(5.6.33) \qquad = \max\{1 - c_0, c_1, \dots, c_{n-1}\}.$$

Now note that

$$(5.6.34) \qquad \sum_{k \in \mathbb{Z}_n} c_k = 1 \implies \sum_{k \neq 0} c_k = 1 - c_0$$

combined with $c_k \geq 0$ we see that

$$(5.6.35) \qquad 1 - c_0 \geq c_k, \quad \forall k > 0,$$

so

$$(5.6.36) \qquad d_\infty(A, C) = 1 - c_0.$$

Similarly, if

$$(5.6.37) \qquad \mathrm{D}(0) = \sum_{r \in \mathbb{Z}_n} d_r |f_r\rangle\langle f_r|,$$

then

$$(5.6.38) \qquad d_\infty(\mathrm{B},\mathrm{D}) = 1 - d_0.$$

5.6.3 Semidefinite program

We can use relations (5.6.36) and (5.6.38), along with (5.6.18) to put constraints on the operator τ we used to define the joint observable

$$(5.6.39) \qquad \sum_h \mathrm{J}(g,h) = \mathrm{C}(g) = U_g \mathrm{C}(0) U_g^\dagger$$

$$(5.6.40) \qquad \frac{1}{n}\sum_h U_g V_h \tau V_h^\dagger U_g^\dagger = U_g \mathrm{C}(0) U_g^\dagger$$

$$(5.6.41) \qquad \iff \frac{1}{n}\sum_h V_h \tau V_h^\dagger = \mathrm{C}(0)$$

$$(5.6.42) \qquad \frac{1}{n}\sum_g U_g \tau U_g^\dagger = \mathrm{D}(0).$$

Computing matrix elements gives

$$(5.6.43) \qquad \langle k|\mathrm{C}(0)|l\rangle = \frac{1}{n}\sum_h \langle k|V_h \tau V_h^\dagger|l\rangle = \frac{1}{n}\sum_h \langle k|V_h^\dagger \tau V_h|l\rangle$$

$$(5.6.44) \qquad = \frac{1}{n}\sum_h \langle k|\tau|l\rangle e^{\frac{2\pi i}{n}h(l-k)}$$

$$(5.6.45) \qquad = \langle k|\tau|l\rangle \delta_{k,l}$$

$$(5.6.46) \qquad \langle f_r|\mathrm{D}(0)|f_s\rangle = \langle f_r|\tau|f_s\rangle \delta_{r,s}.$$

Given that the only matrix elements that affect the uncertainties are the $(0,0)$ matrix element of $\mathrm{C}(0)$ and the (f_0, f_0) matrix element of $\mathrm{D}(0)$ the relevant constraints are

$$(5.6.47) \qquad \langle 0|\tau|0\rangle = 1 - d_\infty(\mathrm{A},\mathrm{C})$$

$$(5.6.48) \qquad \sum_{k,l} \langle k|\tau|l\rangle = n(1 - d_\infty(\mathrm{B},\mathrm{D})).$$

If we set

$$(5.6.49) \qquad A_n = \sum_{k,l} |k\rangle\langle l|$$

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then computing the lower boundary of the uncertainty region is equivalent to the following semidefinite program, for each $d_a \in [0,1]$

(5.6.50)
$$\begin{aligned}
\underset{X}{\text{maximise}} \qquad & p = \text{tr}\,(A_n X) \\
\text{subject to} \quad & \text{tr}\,(|0\rangle\langle 0|X) = 1 - d_a, \\
& \text{tr}\,(\text{I}_n X) = 1, \\
& X \geq 0.
\end{aligned}$$

We can impose the equality constraints in (5.6.50), by means of the linear map

(5.6.51)
$$\mathcal{M} : \mathcal{L}_s(\mathcal{H}) \to M_2(\mathbb{C})$$

(5.6.52)
$$\mathcal{M} : X \mapsto \begin{pmatrix} \text{tr}\,(|0\rangle\langle 0|X) & 0 \\ 0 & \text{tr}\,(X) \end{pmatrix},$$

where $M_2(\mathbb{C})$ is the set of 2 by 2 matrices over the field $\mathbb{C}$. If

(5.6.53)
$$B = \begin{pmatrix} 1 - d_a & 0 \\ 0 & 1 \end{pmatrix}$$

then the equality constraints are

(5.6.54)
$$\mathcal{M}(X) = B$$

We can compute the dual of $\mathcal{M}$ directly from the defining relation

(5.6.55)
$$\text{tr}\,\big(\mathcal{M}^*(Y)X\big) = \text{tr}\,(Y\mathcal{M}(X))$$

(5.6.56)
$$= Y_{00}\,\text{tr}\,(|0\rangle\langle 0|X) + Y_{11}\,\text{tr}\,(\text{I}_n X)$$

(5.6.57)
$$\mathcal{M}^*\left(\begin{pmatrix} Y_{00} & Y_{01} \\ Y_{10} & Y_{11} \end{pmatrix}\right) = Y_{00}|0\rangle\langle 0| + Y_{11}\,\text{I}_n\,.$$

The dual problem to (5.6.50) is then given by

(5.6.58)
$$\begin{aligned}
\underset{Y}{\text{minimise}} \qquad & d = \text{tr}\,(BY) \\
\text{subject to} \quad & \mathcal{M}^*(Y) \geq A_n \\
& Y \in M_2(\mathbb{C}).
\end{aligned}$$

Alternatively

(5.6.59)
$$\begin{aligned}
\underset{y_0,y_1\in\mathbb{R}}{\text{minimise}} \quad & d = (1 - d_a)y_0 + y_1 \\
\text{subject to} \quad & 0 \leq y_0|0\rangle\langle 0| + y_1 \sum_k |k\rangle\langle k| - \sum_{k,l} |k\rangle\langle l| = Z.
\end{aligned}$$

It is easy to see that we have *strong duality* for these problems, since we can always choose y_1 large enough that $Z > 0$, by the Slater condition [71] we therefore know that wherever the solution d to the dual problem is finite we have that $\inf d = \sup p$.

Henceforth we mix operators interchangeably with their matrices in the computational basis. Define the *characteristic polynomial* function for each $n \in \mathbb{N}$

$$(5.6.60) \qquad \chi_n : M_n(\mathbb{C}) \times \mathbb{R} \to \mathbb{R}$$

$$(5.6.61) \qquad \chi_n(X, x) = \det(x\, \mathrm{I}_n - X).$$

We can compute the characteristic polynomial of the matrix Z

$$(5.6.62) \qquad \chi_n(Z, x) = \det(x\, \mathrm{I}_n - Z)$$

$$(5.6.63) \qquad = \det((x - y_1)\mathrm{I}_n - y_0|0\rangle\langle 0| + A_n)$$

$$(5.6.64) \qquad = \det((x - y_1)\mathrm{I}_n + A_n) - y_0\langle 0|\mathrm{adj}((x - y_1)\mathrm{I}_n + A_n)|0\rangle$$

$$(5.6.65) \qquad = \det((x - y_1)\mathrm{I}_n + A_n) - y_0 \det((x - y_1)\mathrm{I}_{n-1} + A_{n-1})$$

$$(5.6.66) \qquad = (-1)^n \det((y_1 - x)\mathrm{I}_n - A_n) - (-1)^{n-1} y_0 \det((y_1 - x)\mathrm{I}_{n-1} - A_{n-1})$$

$$(5.6.67) \qquad = (-1)^n \chi_n(A_n, y_1 - x) + (-1)^n y_0 \chi_{n-1}(A_{n-1}, y_1 - x)$$

$$(5.6.68) \qquad = (-1)^n \left[(x - y_1 - n)(x - y_1)^{n-1} + y_0(x - y_1 - n + 1)(x - y_1)^{n-2} \right]$$

$$(5.6.69) \qquad = (-1)^n (x - y_1)^{n-2} \left[(x - y_1 - n)(x - y_1) - y_0(x - y_1 - n + 1) \right]$$

$$(5.6.70) \qquad = (-1)^n (x - y_1)^{n-2} \left[x^2 + x(n - y_0 - 2y_1) + \left(y_1^2 + y_1(y_0 - n) + y_0(1 - n) \right) \right]$$

where adj denotes the adjudicate matrix, and we have employed the classical matrix determinant lemma, as well as the fact that

$$(5.6.71) \qquad \chi_n(A_n, x) = (x - n)x^{n-1},$$

for A_n the n by n matrix of ones [45]. We are seeking constraints on y_0 and y_1 which are necessary and sufficient for all of the roots of $x \mapsto \chi_n(Z, x)$ to be non-negative, we can read off from (5.6.70) that $y_1 \geq 0$. We now need to examine the roots of

$$(5.6.72) \qquad x \mapsto x^2 + x(n - y_0 - 2y_1) + \left(y_1^2 + y_1(y_0 - n) + y_0(1 - n) \right),$$

the quadratic formula gives

$$(5.6.73) \qquad x^\pm = \frac{1}{2} \left(y_0 + 2y_1 - n \pm \sqrt{(y_0 + 2y_1 - n)^2 - 4(y_1^2 + y_1(y_0 - n) + y_0(1 - n))} \right),$$

note that the roots are automatically real, as our matrices are self-adjoint. The $x^\pm$ are both non-negative if, and only if

$$(5.6.74) \qquad \sqrt{(y_0 + 2y_1 - n)^2 - 4(y_1^2 + y_1(y_0 - n) + y_0(1 - n))} \leq y_0 + 2y_1 - n,$$

which is satisfied if and only if

$$(5.6.75) \qquad 0 \leq y_0 + 2y_1 - n,$$

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and

$$0 \leq y_1^2 + y_1(y_0 - n) + y_0(1 - n), \tag{5.6.76}$$

are both satisfied. The solutions of

$$y_1^2 + y_1(y_0 - n) + y_0(1 - n) = 0 \tag{5.6.77}$$

are

$$y_1^{\pm} = \frac{1}{2}\left(n - y_0 \pm \sqrt{(n - y_0)^2 - 4y_0(1 - n)}\right). \tag{5.6.78}$$

It is easy to show that the radicant is positive. The constraint in (5.6.76) is therefore satisfied if, and only if

$$y_1 \geq \frac{1}{2}\left(n - y_0 + \sqrt{(n - y_0)^2 + 4y_0(n - 1)}\right) \tag{5.6.79}$$

or

$$y_1 \leq \frac{1}{2}\left(n - y_0 - \sqrt{(n - y_0)^2 + 4y_0(n - 1)}\right) \tag{5.6.80}$$

Rewriting (5.6.75) we see we need

$$y_1 \geq \frac{1}{2}(n - y_0), \tag{5.6.81}$$

therefore all of the constraints are satisfied if, and only if

$$y_1 \geq \frac{1}{2}\left(n - y_0 + \sqrt{(n - y_0)^2 + 4y_0(n - 1)}\right), \tag{5.6.82}$$

since the quantity on the right hand side is always positive. Recall that we are attempting to minimise the quantity

$$d = (1 - d_a)y_0 + y_1, \tag{5.6.83}$$

subject to the positivity constraints. We therefore choose

$$y_1 = \frac{1}{2}\left(n - y_0 + \sqrt{(n - y_0)^2 + 4y_0(n - 1)}\right) \tag{5.6.84}$$

$$\implies d = \left(\frac{1}{2} - d_a\right)y_0 + \frac{1}{2}\left(n + \sqrt{(n - y_0)^2 + 4y_0(n - 1)}\right), \tag{5.6.85}$$

differentiating, we find that d is minimised where

$$y_0 = 2 - n - |1 - 2d_a|\sqrt{\frac{n - 1}{d_a(1 - d_a)}}, \tag{5.6.86}$$

and that at this point

$$(5.6.87) \qquad d = 1 + d_a(n-2) + 2\sqrt{d_a(1-d_a)(n-1)}$$

$$(5.6.88) \qquad \implies d_b^{\min} = 1 - \frac{d}{n}$$

$$(5.6.89) \qquad = 1 - \frac{1}{n}\left(1 + d_a(n-2) + 2\sqrt{d_a(1-d_a)(n-1)}\right).$$

We note that this is a section of the ellipse with defining equation

$$(5.6.90) \qquad 0 = n^2 d_a^2 + n^2 d_b^2 + 2n(n-2)d_a d_b + 2n(1-n)d_a + 2n(1-n)d_b + (n-1)^2,$$

which has center $\left(\frac{1}{2}, \frac{1}{2}\right)$, and touches the coordinate axes at the points $\left(0, 1-\frac{1}{n}\right)$ and $\left(1-\frac{1}{n}, 0\right)$. The major axis of the ellipse has angle $\frac{\pi}{4}$ with each coordinate axis, as it must by symmetry.

(a) Hilbert space $\mathscr{H} = \mathbb{C}^2$

(b) Hilbert space $\mathscr{H} = \mathbb{C}^3$

(c) Hilbert space $\mathscr{H} = \mathbb{C}^4$

(d) Hilbert space $\mathscr{H} = \mathbb{C}^6$

(e) Hilbert space $\mathscr{H} = \mathbb{C}^8$

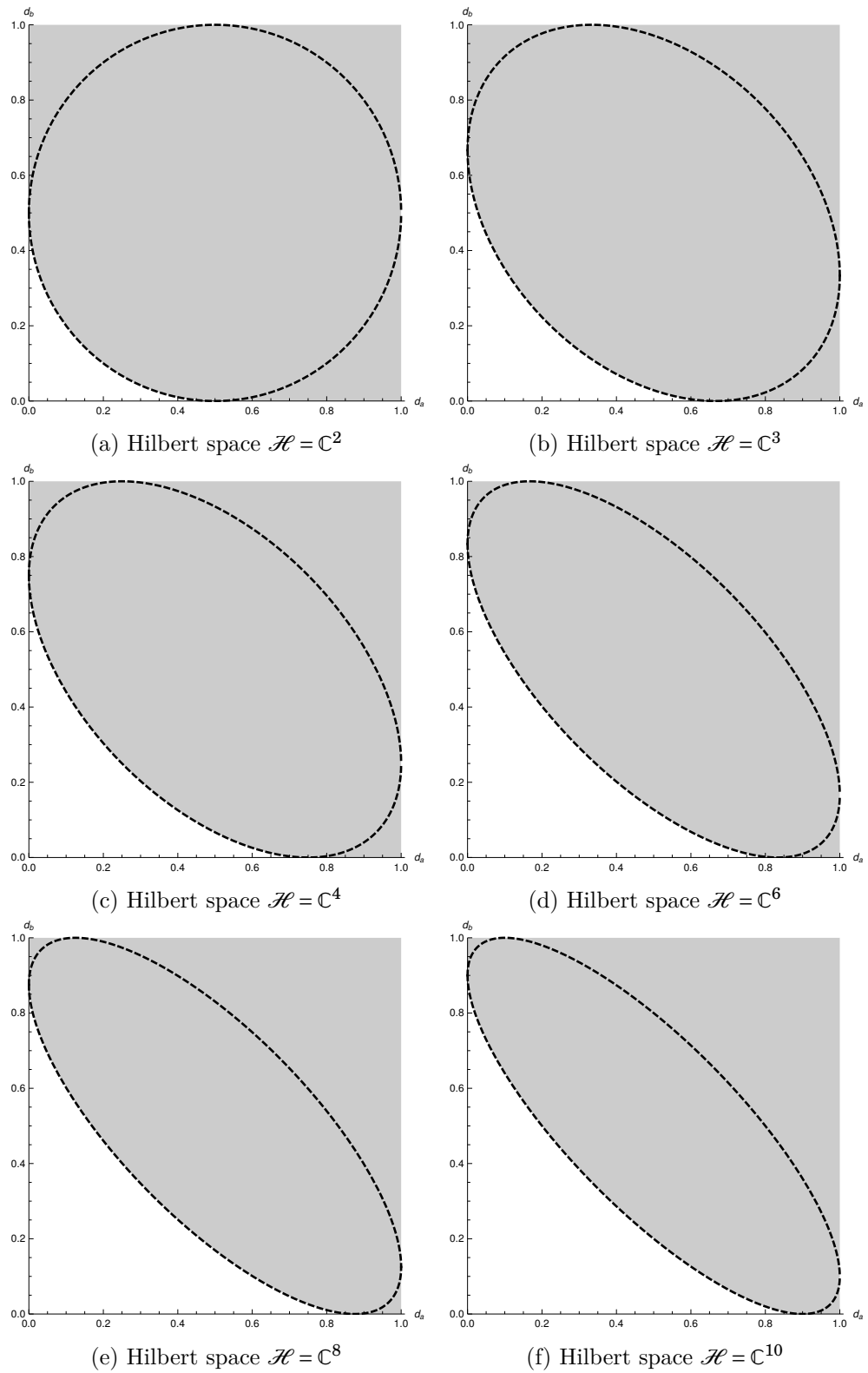(f) Hilbert space $\mathscr{H} = \mathbb{C}^{10}$

Figure 5.3: The measurement uncertainty region for quantum Fourier pair observables in several dimensions.

Conclusions and Outlook

In part I of this thesis we examined preparation uncertainty in both finite and infinite dimensional contexts. We give a new, geometric, derivation of the uncertainty region for sharp ± 1, valued observables. We also provide simple counterexamples demonstrating that the Schrödinger uncertainty relation does not always suffice to fully characterise the uncertainty region for Hilbert spaces of dimension greater than 2. We also compute the uncertainty region for a pair of qutrit observables arising as spectral measures of non-commuting operators, which commute on a subspace, and show that it contains the point where both probability measures are deterministic.

We also examine the preparation uncertainty for the position and momentum observables arising from the well known example of the "particle in a box" system. We compare this with the preparation uncertainty of the free particle, as well as the particle on a ring, previously examined in ref. [13]. The box system lacks the full phase space symmetry which makes the analysis possible for the ring and free particle. Consequently we can not use the methods previously employed to analyse the uncertainty region. Nonetheless we obtain an upper bound on the boundary of the uncertainty and show it is exact in some interval. Explicitly it is exact for position uncertainties greater than some bound. We also show that the well-known canonical hyperbola, attributed to Heisenberg, is a lower bound for the boundary of the uncertainty region and that the difference between the upper and lower bound is small[1], and converges to zero as the position uncertainty becomes small. This reflects the physical intuition that as the states become highly concentrated in position the influence of the boundary conditions becomes less.

An obvious open question is to characterise the uncertainty region in the interval where we

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[1] At the point where they are furthest apart the upper bound is $\frac{1}{2}$ and the lower bound is $\frac{1}{2\sqrt{\frac{\pi^2}{3}-2}} \approx 0.44$

only have upper and lower bounds. We conjecture that the upper bound shown in figure 4.1a is exact globally, rather than just in the region where we have shown it is exact. More strongly, it seems natural to assume that among the states which minimise the momentum uncertainty for a fixed position uncertainty, there are those with position expectation zero. We began analysing the box system as part of a study of preparation uncertainty in the context of multi-slit interferometry. In particular we believe the particle in a box and particle on a ring systems arise if one imposes certain covariance conditions on the which-way and fringe-contrast observables of an idealised infinite interferometer. It would be interesting to explore this further, in particular the physical interpretation of the covariance conditions is not clear. If this can be achieved it might also be interesting to explore alternative covariance conditions.

Little is known about measurement uncertainty in infinite dimensional systems in the absence of the full phase-space symmetry. One could also investigate what could be achieved exploiting only the partial phase-space symmetry exhibited by the "particle in a box" setup.

In part II we provide a systematic framework for exploiting the covariance properties of a family of observables to determine their measurement uncertainty region. This framework may be applied to arbitrary families of finite-outcome observables and a wide class of natural distance measures for observables. Specifically we define a map we call the "invariant mean" which acts as a projection on the space of bounded operator-valued functions on the outcome set. We show that for jointly convex error measures, "compatible" with the symmetry group action, the best compatible approximations to covariant observables are also covariant.

We apply these methods to the case of a metric on observables based on the p-norm, and completely characterise the measurement uncertainty region for a triple of qubit Pauli observables, and for the quantum Fourier pair in arbitrary finite dimensions.

The jointly convex error measures that our framework applies to include the f-divergences introduced in [3] and [26], however the f-divergences may be infinite unless the approximating probability distribution is dominated by the target. If we attempt to follow the previous work and define an f-divergence for quantum observables by taking the supremum over quantum states we will, in general, break this constraint. It might be interesting to characterise the class of functions f for which this does not occur. A reasonable starting point would be those f for which the $\lim_{f \to \infty} f(x) \in \mathbb{R}$, including $f : t \mapsto \frac{1}{t} - 1$, which defines the Neyman divergence.

It would be useful to generalise the invariant mean construction to positive operator valued measures, with infinite outcome sets, for example the canonical position and momentum for a quantum particle. In this case it is not generally possible to express the observable as a simple function from the outcome set. Is not known if the sum over group elements we use to define the invariant mean map may be replaced by a Bochner integral with respect to the Haar measure. Even if the integral is well defined, the resulting quantity may not be an observable.

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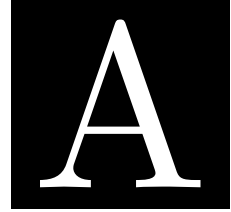
Appendix: Chapter 2

A.1 Example of a non-basis independent "trace"

Consider an infinite dimensional Hilbert space spanned by basis vectors $\{|e_k\rangle | k \in \mathbb{N}\}$. Let Z be the operator acting as

$$(A.1.1) \qquad Z|e_{2n}\rangle = |e_{2n}\rangle$$

$$(A.1.2) \qquad Z|e_{2n+1}\rangle = -|e_{2n+1}\rangle,$$

effectively the direct sum of Pauli-z operators acting in two dimensional subspaces. For $k \in \mathbb{N}$ define the operators $U_{k\theta}$ acting as rotations around the y axis in the kth two dimensional subspace, and the identity outside

$$(A.1.3) \qquad U_{k\theta}|e_{2k}\rangle = \cos(\theta)|e_{2k}\rangle + \sin(\theta)|e_{2k+1}\rangle$$

$$(A.1.4) \qquad U_{k\theta}|e_{2k+1}\rangle = -\sin(\theta)|e_{2k}\rangle + \cos(\theta)|e_{2k+1}\rangle$$

$$(A.1.5) \qquad U_{k\theta}|e_k\rangle = |e_j\rangle,$$

where $j \neq 2k, 2k+1$, then

$$(A.1.6) \qquad \langle U_{k\theta}e_{2k}|ZU_{k,\theta}e_{2k}\rangle = \cos^2(\theta) - \sin^2(\theta)$$

$$(A.1.7) \qquad \langle U_{k\theta}e_{2k+1}|ZU_{k,\theta}e_{2k+1}\rangle = -\cos^2(\theta) + \sin^2(\theta).$$

We choose θ_k such that

$$(A.1.8) \qquad \langle U_{k\theta_k}e_{2k}|ZU_{k,\theta_k}e_{2k}\rangle = \frac{1}{k+1} = -\langle U_{k\theta_k}e_{2k+1}|ZU_{k,\theta_k}e_{2k+1}\rangle.$$

If the basis $\{|\phi_k\rangle \,|\, k \in \mathbb{N}\}$ is chosen such that

$$(A.1.9) \qquad\qquad |\phi_{2k}\rangle = U_{k,\theta_k} e_{2k}$$

$$(A.1.10) \qquad\qquad |\phi_{2k+1}\rangle = U_{k,\theta_k} e_{2k+1},$$

then we can rewrite the terms of the series

$$(A.1.11) \qquad\qquad \sum_{k \geq 0} \langle \phi_k | Z \phi_k \rangle = \sum_{k > 0} \frac{(-1)^{k-1}}{\lfloor k/2 \rfloor},$$

where $\lfloor x \rfloor$ denotes the *floor* of x, the largest natural below x. It is now easy to see the series converges to zero, but does not converge absolutely. By the Riemann series theorem [77] this series may be rearranged (by relabelling basis elements) to give any real number as the sum.

B

Appendix: Chapter 3

B.1 Uncertainty region for Gell-Mann observables

Given

$$
\text{(B.1.1)} \qquad A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \rho = \begin{pmatrix} \rho_{11} & 0 & \rho_{13} \\ 0 & 1 - \rho_{11} - \rho_{33} & 0 \\ \rho_{13}^{*} & 0 & \rho_{33} \end{pmatrix},
$$

we can solve

$$
\text{(B.1.2)} \qquad x = \Delta_{\rho}^{2} A
$$
$$
\text{(B.1.3)} \qquad = 1 - \rho_{33} - \left(2\rho_{11} + \rho_{33} - 1\right)^{2},
$$

giving

$$
\text{(B.1.4)} \qquad \rho_{33}^{\pm} = \frac{1}{2}\left(1 - 4\rho_{11} \pm \sqrt{1 + 8\rho_{11} - 4x}\right).
$$

The positivity of ρ constrains the choice of ρ_{11} values in each case. If

$$
\text{(B.1.5)} \qquad \rho^{\pm} = \begin{pmatrix} \rho_{11} & 0 & \rho_{13} \\ 0 & 1 - \rho_{11} - \rho_{33}^{\pm} & 0 \\ \rho_{13}^{*} & 0 & \rho_{33}^{\pm} \end{pmatrix}
$$

and $0 \le \rho_{13} \le \sqrt{\rho_{11}\rho_{33}}$ then

(B.1.6)

$$\rho^+ \ge 0 \iff \begin{cases} \left[0 \le \rho_{11} \le \frac{1}{2}(1-\sqrt{1-4x})\right] \text{ or } \left[\frac{1}{2}(1+\sqrt{1-4x}) \le \rho_{11} \le \frac{1}{2}(1+\sqrt{1-x})\right], & 0 \le x \le \frac{1}{4} \\ \frac{1}{8}(4x-1) \le \rho_{11} \le \frac{1}{2}\left(1+\sqrt{1-x}\right), & \frac{1}{4} \le x \le \frac{3}{4} \\ \frac{1}{2}\left(1-\sqrt{1-x}\right) \le \rho_{11} \le \frac{1}{2}(1+\sqrt{1-x}), & \frac{3}{4} \le x \le 1 \end{cases}$$

(B.1.7)

$$\rho^- \ge 0 \iff \begin{cases} 0 \le \rho_{11} \le \frac{1}{2}(1-\sqrt{1-x}), & 0 \le x \le \frac{1}{4} \\ \frac{1}{8}(4x-1) \le \rho_{11} \le \frac{1}{2}(1-\sqrt{1-x}), & \frac{1}{4} \le x \le \frac{3}{4} \\ \text{no valid solution}, & \frac{3}{4} \le x \le 1. \end{cases}$$

The constraints on ρ_{13} imply that $0 \le \left(\text{Re}\,\rho_{13}\right)^2 \le \rho_{11}\rho_{33}^\pm$. Obviously $\Delta_{\rho^\pm}^2 \mathbf{B}$ will be minimised by a $\rho^\pm$ with $\left(\text{Re}\,\rho_{13}\right)^2 = \rho_{11}\rho_{33}^\pm$ and maximised when $\left(\text{Re}\,\rho_{13}\right)^2 = 0$.

(B.1.8)
$$\Delta_{\rho^\pm}^2 \mathbf{B} = \rho_{11} + \rho_{33}^\pm - 4\lambda\rho_{11}\rho_{33}^\pm.$$

For a fixed x the local minima and maxima will either be where the inequalities above are saturated or where the derivative of $\Delta_{\rho^\pm}^2 \mathbf{A}$ with respect to ρ_{11} (considering $\rho_{33}^\pm$ as a function of ρ_{11}) is zero.

B.1.1 Exploring minima

Here we consider the case $\left(\text{Re}\,\rho_{13}\right)^2 = \rho_{11}\rho_{33}^\pm$. In this case

(B.1.9)
$$\Delta_{\rho^\pm}^2 \mathbf{B} = \rho_{11} + \rho_{33}^\pm - 4\rho_{11}\rho_{33}^\pm$$

(B.1.10)
$$= \frac{1}{2}\left(1 - 6\rho_{11} + 16\rho_{11}^2 \pm (1-4\rho_{11})\sqrt{1+8\rho_{11}-4x}\right)$$

(B.1.11)
$$\frac{\mathrm{d}\left(\Delta_{\rho^\pm}^2 \mathbf{B}\right)}{\mathrm{d}\rho_{11}} = -3 + 16\rho_{11} \mp 2\sqrt{1+8\rho_{11}-4x} \pm \frac{2-8\rho_{11}}{\sqrt{1+8\rho_{11}-4x}}$$

(B.1.12)
$$\frac{\mathrm{d}\left(\Delta_{\rho^\pm}^2 \mathbf{B}\right)}{\mathrm{d}\rho_{11}} = 0 \iff (3-16\rho_{11})\sqrt{1+8\rho_{11}-4x} = \pm\left(8x-24\rho_{11}\right).$$

The solutions to this equation obey a cubic equation

(B.1.13)
$$(3-16\rho_{11})^2(1+8\rho_{11}-4x) = \left(8x-24\rho_{11}\right)^2$$

(B.1.14)
$$0 = (32\rho_{11}-16x+3)(8\rho_{11}(8\rho_{11}-5)+4x+3),$$

with solutions

(B.1.15)
$$\rho_{11}^\pm = \frac{1}{16}\left(5 \pm \sqrt{13-16x}\right)$$

(B.1.16)
$$\rho_{11}^0 = \frac{1}{32}(16x-3).$$

Substituting these back into (B.1.12) we see that ρ_{11}^0 and ρ_{11}^+ are solutions wherever they give valid quantum states, but ρ_{11}^- is only a solution if $x = \frac{9}{16}$ or $\frac{3}{4} \le x$. Comparing the solutions with the restrictions (B.1.6) we get the following solutions for ρ^+, and no solutions for ρ^-

$$(B.1.17a) \qquad \rho_{11} = \frac{1}{32}(16x - 3) \text{ on } x \in \left[\frac{3}{16}, \frac{15}{16}\right]$$

$$(B.1.17b) \qquad \rho_{11} = \frac{1}{16}\left(5 + \sqrt{13 - 16x}\right) \text{ on } x \in \left[\frac{9}{100}, \frac{13}{16}\right]$$

$$(B.1.17c) \qquad \rho_{11} = \frac{1}{16}\left(5 - \sqrt{13 - 16x}\right) \text{ on } x \in \left\{\frac{9}{16}\right\} \cup \left[\frac{3}{4}, \frac{13}{16}\right],$$

note that the apparently exceptional point $x = \frac{9}{16}$, $\rho_{11} = \frac{3}{16}$ lies on the line $\rho_{11} = \frac{1}{32}(16x - 3)$. To these we add the boundary values

$$(B.1.18a) \qquad \rho_{11} = 0 \text{ with } \rho_{33}^+ \text{ and } x \in \left[0, \frac{1}{4}\right]$$

$$(B.1.18b) \qquad \rho_{11} = \frac{1}{2}\left(1 - \sqrt{1 - 4x}\right) \text{ with } \rho_{33}^+ \text{ and } x \in \left[0, \frac{1}{4}\right]$$

$$(B.1.18c) \qquad \rho_{11} = \frac{1}{2}\left(1 + \sqrt{1 - 4x}\right) \text{ with } \rho_{33}^+ \text{ and } x \in \left[0, \frac{1}{4}\right]$$

$$(B.1.18d) \qquad \rho_{11} = \frac{1}{2}\left(1 + \sqrt{1 - x}\right) \text{ with } \rho_{33}^+ \text{ and } x \in [0, 1]$$

$$(B.1.18e) \qquad \rho_{11} = \frac{1}{8}(4x - 1) \text{ with } \rho_{33}^+ \text{ and } x \in \left[\frac{1}{4}, \frac{3}{4}\right]$$
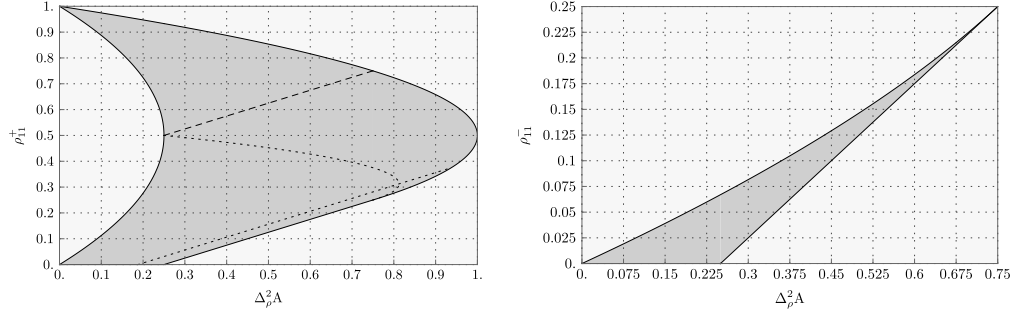
$$(B.1.18f) \qquad \rho_{11} = \frac{1}{2}\left(1 - \sqrt{1 - x}\right) \text{ with } \rho_{33}^+ \text{ and } x \in \left[\frac{3}{4}, 1\right]$$

$$(B.1.18g) \qquad \rho_{11} = 0 \text{ with } \rho_{33}^- \text{ and } x \in \left[0, \frac{1}{4}\right]$$

$$(B.1.18h) \qquad \rho_{11} = \frac{1}{8}(4x - 1) \text{ with } \rho_{33}^- \text{ and } x \in \left[\frac{1}{4}, \frac{3}{4}\right]$$

$$(B.1.18i) \qquad \rho_{11} = \frac{1}{2}(1 - \sqrt{1 - x}) \text{ with } \rho_{33}^- \text{ and } x \in \left[0, \frac{3}{4}\right]$$

the (locally) extremising values of ρ_{11} are summarised in Figure B.1a. The values of $\Delta^2_{\rho_{11}^+} B$ given these choices of ρ_{11}, and $\left(\text{Re}\,\rho_{13}\right)^2 = \rho_{11}\rho_{33}^\pm$ are plotted in Figure B.1b.

(a) Range of ρ_{11} given $\rho_{33} = \rho_{33}^+$. The dotted lines are the where $\text{Re}\,\rho_{13}$ is maximal and the derivative of $\Delta_{\rho^+}^2 B$ with respect to ρ_{11} is zero (B.1.17), the dashed line is the where $\text{Re}\,\rho_{13} = 0$ and the derivative of $\Delta_{\rho^+}^2 B$ with respect to ρ_{11} is zero (B.1.23).

(b) Range of ρ_{11} given $\rho_{33} = \rho_{33}^-$. There are no local extrema other than the boundary curves.

Figure B.1: The filled region indicates the allowed values of ρ_{11} as a function of $\Delta_{\rho^+}^2 A$ in each case. The solid lines are the boundary curves, given in (B.1.18).

B.1.2 Exploring maxima

Here we consider the case $\left(\text{Re}\,\rho_{13}\right)^2 = 0$. In this case

$$\Delta_{\rho^\pm}^2 B = \rho_{11} + \rho_{33}^\pm \tag{B.1.19}$$

$$= \frac{1}{2}\left(1 - 2\rho_{11} \pm \sqrt{8\rho_{11} - 4x + 1}\right) \tag{B.1.20}$$

$$\frac{\mathrm{d}\left(\Delta_{\rho^\pm}^2 B\right)}{\mathrm{d}\rho_{11}} = -1 \pm \frac{2}{\sqrt{8\rho_{11} - 4x + 1}} \tag{B.1.21}$$

$$\frac{\mathrm{d}\left(\Delta_{\rho^\pm}^2 B\right)}{\mathrm{d}\rho_{11}} = 0 \iff \sqrt{8\rho_{11} - 4x + 1} = \pm 2. \tag{B.1.22}$$

There are no solutions for ρ_{33}^-, but ρ_{33}^+ has the solution

$$\rho_{11} = \frac{1}{8}(3 + 4x), \tag{B.1.23}$$

which is always a valid solution for ρ^+ and never valid for ρ^-. To this we add the boundary values which are the same as those with $\left(\text{Re}\,\rho_{13}\right)^2 = \rho_{11}\rho_{33}$, given in (B.1.18).

B.1.3 The bounding curves

Comparing the local extrema we can now describe the full uncertainty region shown in figure 3.9

$$(B.1.24) \qquad \Delta^2 B = 1, \qquad \Delta^2 A \in \left[0, \frac{1}{4}\right]$$

$$(B.1.25) \qquad \Delta^2 B = \frac{1}{8}\left(9 - 4\Delta^2 A\right), \qquad \Delta^2 A \in \left[\frac{1}{4}, \frac{3}{4}\right]$$

$$(B.1.26) \qquad \Delta^2 B = \frac{1}{2}\left(1 + \sqrt{1 - \Delta^2 A}\right), \qquad \Delta^2 A \in \left[\frac{3}{4}, 1\right]$$

$$(B.1.27) \qquad \Delta^2 B = \frac{1}{2}\left(1 - \sqrt{1 - \Delta^2 A}\right), \qquad \Delta^2 A \in \left[\frac{15}{16}, 1\right]$$

$$(B.1.28) \qquad \Delta^2 B = 2\left(\Delta^2 A\right)^2 - \frac{11}{4}\Delta^2 A + \frac{153}{128} \qquad \Delta^2 A \in \left[\frac{13}{16}, \frac{15}{16}\right]$$

$$(B.1.29) \qquad \Delta^2 B = \frac{1}{8}\left(4\Delta^2 A - 1\right), \qquad \Delta^2 A \in \left[\frac{1}{4}, \frac{13}{16}\right]$$

$$(B.1.30) \qquad \Delta^2 B = 1 - \Delta^2 A, \qquad \Delta^2 A \in \left[\frac{15}{64}, \frac{1}{4}\right]$$

$$(B.1.31) \qquad \Delta^2 B = \frac{1}{2}\left(1 - \sqrt{1 - \Delta^2 A}\right) \qquad \Delta^2 A \in \left[0, \frac{15}{64}\right]$$

$$(B.1.32) \qquad \Delta^2 B = \frac{1}{2}\left(1 - \sqrt{1 - 4\Delta^2 A}\right) \qquad \Delta^2 A \in \left[0, \frac{3}{16}\right]$$

$$(B.1.33) \qquad \Delta^2 B = 1 - 4\Delta^2 A, \qquad \Delta^2 A \in \left[0, \frac{3}{16}\right].$$