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D.A. Dubin & M.A. Hennings

Quantum mechanics, algebras and distributions

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Quantum mechanics, algebras and distributions

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This book is dedicated to

OUR TEACHERS

with thanks

1. INTRODUCTION

Both quantum mechanics and statistical mechanics share the notable property that an understanding of the theory lies rather deep, yet a mastery of the associated calculations is quite straightforward. Moreover, it is perfectly reasonable to do research in either subject without usually considering the difficult problems underlying the theory. It is unfortunate that this circumstance fosters the idea that such problems as there may be are irrelevant to anything important.

The problems we have in mind do not admit of easy solutions. A necessary prerequisite to progress is a careful and rigorous formulation. This will at least separate the essential from the inessential difficulties. It will also make it difficult to believe that there are no problems.

These notes have as their goal a mathematically precise formulation of elementary quantum mechanics, based on the considerations of the following paragraphs.

The basic observables in quantum mechanics, such as position, momentum, energy and angular momentum, are represented by unbounded linear operators on some Hilbert space. These operators can have both discrete and continuous components to their spectra, necessitating a consistent scheme to take this into account.

A consistent scheme requires, firstly, an explicit choice of domain, common to all observables. This condition follows from two considerations. One, that the observables constitute an algebra reflecting the canonical commutation relations. Two, that the measured values of any observable in any state be finite. This last requirement we term the basic measurement principle.

The canonical commutation relations (ccr) are the equations of noncommutativity between the coordinate and momentum operators. For one degree of freedom there is only one equation,

$$qp - pq = i\hbar. \tag{1.1}$$

The measure of noncommutativity is Planck's constant,

$$\hbar = 1.0545 \times 10^{-27}\,\mathrm{erg\,sec.}$$

and equation (1.1) encapsulates the essential difference between quantum and classical mechanics. (Born and Jordan [1], Born, Jordan and Heisenberg [1], Dirac [1-2], Heisenberg [1-3].)

Any mathematical theory which proposes to deal with q and p directly, must logically begin with an analysis of the representations of equation (1.1). In Theorem [2.4] below, we learn that q and p cannot both be bounded. As in the modern theory of partial differential equations, this leads us to consider them as continuous linear operators on certain locally convex spaces, or *lcs* for short. For interpretative purposes, these spaces will have to be continuously and densely embedded in Hilbert spaces.

As a purely mathematical problem, there are many inequivalent representations of the *ccr*, typically of no clear physical significance. For this reason, we impose the following physical constraint : a representation is allowable if and only if it contains what we term a gauge invariant state.

To explain : let T be a state of the system. Let a be an observable, and let $T(a)$ indicate the relevant duality pairing. We take it as axiomatic that when an observable a is measured in the state T, a statistical distribution of results is obtained : the $T(a^n)$ are the moments of a probability measure. We shall consider this at length in Chapter 7. Granting this, $T(a)$ is the expected, or mean, value, and $[T(a^2) - T(a)^2]^{1/2}$ is the the standard deviation, written $\Delta_T(a)$.

It is an elementary calculation that for any state T, equation (1.1) leads to the Heisenberg uncertainty relations for the standard deviations of the position and momentum operators (Bohm [1], Heisenberg [2], Thirring [1]):

$$\Delta_T(q)\,\Delta_T(p) \geq \hbar/2. \tag{1.2}$$

The physical consequences of this are important and far reaching. For an analysis of the principal consequences, see Heisenberg [2]. Hereafter we employ units such that $\hbar = 1$ unless this would obscure a physical argument.

Coming back to our physically motivated condition on the representations of the *ccr*, it is equivalent to the existence of a state T such that the means vanish:

$$T(q) = T(p) = 0, \tag{1.3.a}$$

and the standard deviations are equal and minimal:

$$\Delta_T(q) = \Delta_T(p) = 2^{-1/2}. \tag{1.3.b}$$

The reason for the name gauge invariance is that equation (1.3) is equivalent to the invariance of T under the following action of the circle group:

$$\Gamma_\theta = \exp\left[i\theta(p^2 + q^2 - 1)/2\right], \qquad (0 \leq \theta < 2\pi). \tag{1.4.a}$$

That is,

$$T \circ \Gamma_\theta = T, \qquad (0 \leq \theta < 2\pi). \tag{1.4.b}$$

Because Γ bears a certain formal resemblance to the gauge group of quantum statistical mechanics and the gauge transformations of electromagnetism, we call it the gauge group in this context as well.

Granting this condition, we may invoke a theorem of Kristensen, Mjelbo and Thue–Poulsen [1], which we prove as Theorem [2.19] below. This tells us that all complete irreducible such representations are equivalent to the representation found by Schrödinger in his theory of wave mechanics [1–4].

The carrier space for the Schrödinger representation is the nuclear Fréchet space $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ of smooth functions of rapid decrease (Trèves [1]). In this representation it is possible to identify the position and momentum operators as the generators of momentum and space translations, respectively.

It is interesting and important that $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ is precisely the domain common to all polynomials in these operators. For this reason we refer to functions in $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ as *wave functions* and $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ itself as the space of wave functions. Similarly, we refer to any unitarily equivalent carrier space as a space of wave functions, and write $\mathcal{W}$ for a generic representative.

The nonrelativistic Pauli theory of spin and statistics can be included by considering $\mathcal{S}\left(\mathbb{R}^{3N}; \mathbb{C}^{2s+1}\right)$ and its symmetric and antisymmetric subspaces (Pauli [1-3]). Several types of particles may be considered by combining these latter spaces by means of tensor products. Finally, one may wish to consider reducible representations. These are direct sums of the above spaces. At the end we have a nuclear Fréchet space $\mathcal{W}$ of wave functions.

The next stage of the theory requires a choice of the algebra of observables, $\mathcal{A}$. We take the largest natural candidate, which is the set $\mathcal{L}^{+}(\mathcal{W})$ of continuous linear operators on $\mathcal{W}$ which have adjoints under which $\mathcal{W}$ is stable.

The construction of $\mathcal{W}$ is such that it is part of a rigged triple (Gel'fand and Vilenkin [1], Maurin [1]):

$$\mathcal{W} \subset \mathcal{H} \subset \mathcal{W}'.$$

In the case where $\mathcal{W} = \mathcal{S}\left(\mathbb{R}^{3N}\right)$, $\mathcal{H}$ is $L^2\left(\mathbb{R}^{3N}\right)$ and $\mathcal{W}'$ is the space of tempered distributions. The adjoint of an operator on $\mathcal{W}$ is meant in the usual Hilbert space sense. It is an essential complication of the theory that there are operators in $\mathcal{L}(\mathcal{W})$, the space of continuous linear operators on $\mathcal{W}$, which have adjoints under which $\mathcal{W}$ is not stable. Having chosen those operators for which this is not the case, we write a^{+}

for the adjoint restricted to $\mathcal{W}$,

$$a^+ = a^*|_{\mathcal{W}}.$$

Once $\mathcal{A}$ has been chosen, it is possible to analyze its algebraic and topological properties, and we shall do so. The next theme that occurs is positivity. It turns out to be best to define an element of $\mathcal{A}$ to be positive if it is positive in the usual Hilbert space sense. That is, if

$$\langle x, ax \rangle \geq 0, \qquad x \in \mathcal{W}.$$

The set of all such operators is a proper cone in $\mathcal{A}$, and as such defines an order relation. The connection between the topology on $\mathcal{A}$ and this order relation is strong, as the original topology will be shown to be the order topology constructed from the cone.

As we are dealing with tempered distributions, it is not difficult to obtain a kernel representation for the observables. This is an injection $a \to A$ of $\mathcal{A}$ into $\mathcal{W}'\widehat{\otimes}\mathcal{W}'$. For the Schrödinger representation, the kernel is determined from

$$af(x) = \int_{\mathbb{R}^{3N}} A(x,y)f(y), \qquad f \in \mathcal{S}\left(\mathbb{R}^{3N}\right).$$

The identity operator, for example, has the Dirac delta distribution as its kernel. Other cases are similarly defined.

The kernel representation is useful for the analysis of the space $\mathcal{A}'$ of continuous linear functionals on $\mathcal{A}$. In fact, $\mathcal{A}'$ turns out to be identifiable with the function space $\mathcal{W}\widehat{\otimes}\mathcal{W}$. A careful analysis then shows that elements of $\mathcal{A}'$ may also be identified with trace class operators ρ on $\mathcal{H}$ such that $a\rho b$ and $a\rho^* b$ are trace class for all observables a, b. We call these $\mathcal{W}$-nuclear operators.

In this last identification, the positive functionals are those ρ which are also positive operators on $\mathcal{H}$. If we then define states on $\mathcal{A}$ to be positive functionals in $\mathcal{A}'$ which are normalized on the unit operator, they are positive $\mathcal{W}$-nuclear operators ρ with

$$\operatorname{tr} \rho = 1;$$

these are known to physicists as density matrices.

As the set of states is convex, it possesses extreme points. From the density matrix representation it is easy to show that these are in one to one correspondence with the points of $\mathcal{W}$.

This is very satisfactory. On general physical principles we want general (mixed) states to be convex combinations of wave functions, and this is what occurs. In the model where the algebra of observables is $\mathcal{L}(\mathcal{H})$, for example, this is not the case. Only functionals satisfying an additional continuity condition (normality) are traces.

It is worth emphasizing that $(\mathcal{W}, \mathcal{A})$ is self–referential in the following sense. Suppose we were given $\mathcal{A}$ before we knew what $\mathcal{W}$ was. We could still define the states as normalized positive functionals on $\mathcal{A}$. The pure states would then determine $\mathcal{W}$.

This is a noncommutative version of the situation pertaining to smooth manifolds. Starting from the algebra of smooth functions, the manifold is the set of extreme states on the algebra. This point of view has been emphasized by Connes as a version of noncommutative differential geometry. An area where this may prove useful is in some recent gauge/string theories in physics, where the spacetime points are to be secondary constructions.

The second requirement for consistency is a reworking of the theory of measurement, within the Copenhagen interpretation, but varied so as to be compatible with the algebraic framework.

The analysis of the measurement process presents some novel features as well. Our notion of measurement is based on the existence of instruments. These devices test incoming states for various quantum properties, and then emit output states contingent upon the results observed.

Mathematically, an instrument is a linear map on the set of states, obeying the modest requirements of continuity and countable additivity with respect to the spectrum of the observable it represents.

Consider those observables with empty essential spectrum, and whose eigenvectors are in the common domain. A measurement will necessarily produce an eigenvalue only, and the output state is then that eigenstate. Immediate remeasurement using the eigenstate as input will reproduce the same eigenvalue and eigenstate surely. This illustrates the collapse of the wave packet and strict repeatability.

Such observables constitute only a small part of the algebra, and the position, momentum and energy are not amongst them. For the general observable we find that completely accurate instruments do not exist. Moreover, only partial information about the observable may be obtainable. Different nonideal measurements must be pieced together to maximize the information about an observable.

More arresting is the fact that there is no strict repeatability in general. As there are no eigenvectors for the continuous spectrum, this ought not to be so surprising. This phenomenon has to do with the essential spectrum and not the boundedness. Davies and Lewis [1] have noted this for such cases.

It is in order here to consider in what respects our treatment differs from that of other authors. At the outset we choose to examine only the mathematical structure of the theory; we do not consider any detailed physical situations. We also consider the model based on unbounded operators exclusively. In this way we follow the path laid out in Dirac's book [2]. There are two principal differences from that text. The first is our strong emphasis on the algebraic aspect. The second is that we use the full apparatus of the theory of topological vector spaces, which was not available to Dirac.

The typical reader we have in mind should have a basic knowledge of the theory of locally convex spaces. The book of Robertson and Robertson [1] is what we have in mind. Although not absolutely necessary, it would put matters in context if the reader has met quantum mechanics before, in some version or another. If not, the reader will find occasional remarks scattered throughout the notes providing a simple orientation towards the physics.

For physicists who have not met locally convex spaces before, we suggest working backwards from the axioms, considering only as much of the mathematics as seems reasonable. We have gathered the axioms together at the end of Chapter 7.

We should like to end this introduction by writing down von Neumann's axiom scheme for quantum mechanics. These are based on the choice of bounded operators as observables. In [2.27] below, we shall briefly consider a C^*-algebra version of the bounded operator model. For now, the following list will serve for contrast with the model to be discussed in the succeeding chapters.

1: To every system there corresponds a Hilbert space $\mathcal{H}$. Normalized elements of $\mathcal{H}$ are the pure states of the system. Impure states are positive normalized trace class operators.

2: Observables are represented by self adjoint operators on $\mathcal{H}$.

3: Time translations of the states are effected by the unitary group whose generator is the Hamiltonian operator, which is the energy observable.

4: If the observable a is measured when the system is in the state ρ, the probability that a value in the range $\Delta \subseteq \mathbb{R}$ is obtained is

$$\operatorname{tr}[\rho P(\Delta)]. \tag{1.5}$$

Here P is the projection valued measure of the spectral decomposition of a.

5: If the observable a has a simple discrete spectrum,

$$a = \sum_n \alpha_n P_n,$$

then immediately upon the observation of a value α_n, the state collapses $\rho \to P_n$.

6: For N point particles moving in space, the representation obtained by Schrödinger in his wave mechanics is appropriate. This is the representation in which the position operators are all diagonalized as multiplication operators on $L^2\left(\mathbb{R}^{3N}\right)$.

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2. BASIC QUANTUM MECHANICS

2.1 ELEMENTARY QUANTUM SYSTEMS

Our concern in these notes is with a mathematical model describing nonrelativistic atomic and molecular phenomena. To be precise, we propose to discuss the following class of systems.

Axiom 1. By an elementary quantum system we mean an assemblage consisting of a fixed finite number N of particles moving nonrelativistically in space $\mathbb{R}^3$ under the influence of their mutual potentials and any external potentials present. These particles are electrons, protons and neutrons or bound aggregates of them. The invariant attributes of such a particle are its mass, charge and spin, and that to a good approximation it may be treated as a point particle. The number $d = 3N$ is known as the number of degrees of freedom of the system. When there is no possible ambiguity, we shall write Σ_d for an elementary quantum system with d degrees of freedom. ■

We wish to emphasize our choice of $\mathbb{R}^3$ as the co-ordinate configuration space. Fundamentally there are no infinite barriers or wells, atomic particles do not move in one dimension or on the surface of a torus, and so on. These are idealizations which focus attention on the physically important features of the process, and are computationally useful. But idealizations they are, and in principle are contained in the full theory.

We shall not consider nuclear effects, relativity, or any high energy phenomena. This puts a lower limit to the scale of distances considered, roughly 10^{-8} centimetres. At the other extreme, we shall not consider molecular or chemical phenomena save indirectly.

The material atomic entities, electrons, protons and neutrons, are incredibly small: if a drop of water is imagined to be magnified to the size of the earth, with all its components proportional, then an atom will have a diameter of a few metres and a nucleus a diameter of less than 1/100 of a millimetre. As for their weight, 10^{28} electrons have a combined mass of less than a gram.

It is extremely important to realize that we have no direct sensory experience of such objects. All our knowledge of these particles is based on inference from their interactions with macroscopic measuring and recording devices. There is a very natural temptation to organize our description of atomic phenomena in macroscopic terms, such as waves or particles. To do so is to guarantee physical and logical inconsistency (Bohr [2-3]).

2.2 STATES AND OBSERVABLES

The undefined notions in quantum physics are states and observables. The dictionary definition of a state may be paraphrased as *the instantaneous condition in which the system is*. All the information obtainable concerning the condition is inherent in the state.

One of the crucial aspects of quantum theory concerns the definiteness of that information, for there exist states which correspond to indefinite values of the dynamical quantities, such as energy. Analysis shows that such states may be represented as convex combinations of states with definite values: in this sense the system can be in two or more states of, say, definite energy at the same time. Along with this indefiniteness there is an inherent uncertainty as to the value that will be obtained when a dynamical variable is measured and the system is in such a state. States, then, have a physical interpretation that introduces probability and indeterminacy.

The other primitive notion is that of observable. This must formalize the quantum analogues of the classical dynamical variables at a given time, such as position, momentum, energy, and the like. It is a postulate of the theory that the observables are elements of an algebra and the states are linear functionals. In the terminology of Lassner and Uhlmann [1], quantum mechanics is an observer–state system.

2.1 Definition An observer–state system is a pair $(\mathcal{A}, \mathtt{S})$, where $\mathcal{A}$ is a complex *–algebra with an identity $\mathbf{1}$, and $\mathtt{S}$ is the convex set of positive normalized linear functionals on $\mathcal{A}$. We refer to $\mathcal{A}$ as the algebra of observables and $\mathtt{S}$ as the set of states. That is, a state is a linear map $T : \mathcal{A} \to \mathbb{C}$ such that

$$T(\mathbf{1}) = 1 \qquad \text{and} \qquad T(x^*x) \geq 0$$

for all $x \in \mathcal{A}$. ■

We shall define and analyze these notions further in the next chapter. Two very convenient conventions of terminology will now be instituted. The first is the identification of the dynamic variables with the operators that represent them, both being termed observables. The second is to extend the term observable to cover all elements of the algebra of observables. This leaves open the question of precisely which observables are physically observable. We shall answer this question in the chapter on the theory of measurements. Suffice it to say that it is a subset of the hermitian elements, *ie* , elements that satisfy $x = x^*$, possibly proper.

One of the requirements of the theory is a choice of algebra. We follow Dirac [2] in requiring the observable algebra to contain all the quantum analogues of the dynamical variables of classical mechanics. Ignoring spin for the time being, this means that the algebra contains operators that satisfy the canonical commutation relations. In fact it will turn out that such operators generate the observable algebra in a certain sense. It is important, therefore, to determine what constraints this places on the theory.

2.3 REPRESENTATIONS OF THE *CCR*

We take this opportunity to introduce our multi–index notation, which will be used throughout these notes.

2.2 Notation Given $\mathbf{x} \in \mathbb{R}^d$, we write $\mathbf{x} = (x_1, \ldots, x_d)$ for its components. The corresponding partial derivatives are denoted

$$\partial/\partial\mathbf{x} = (\partial/\partial x_1, \ldots, \partial/\partial x_d).$$

Integral exponents require d–tuples $\mathbf{n} = (n_1, \ldots, n_d)$ in $\mathbb{N}^d$, and we write

$$\mathbf{x}^{\mathbf{n}} = x_1^{n_1} \cdots x_d^{n_d};$$

similarly for $(\partial/\partial\mathbf{x})^{\mathbf{n}}$.

Unless otherwise specified we use the Euclidean norm for $\mathbf{x} \in \mathbb{R}^d$, writing

$$\|\mathbf{x}\|^2 = |x_1|^2 + \cdots + |x_d|^2;$$

and the l^1–norm for $\mathbb{N}^d$:

$$|\mathbf{n}| = |n_1| + \cdots + |n_d|.$$

Real multinomials are written as

$$|\mathbf{x}|^{\mathbf{n}} = |x_1|^{n_1} \cdots |x_d|^{n_d},$$

and multi-factorials as

$$\mathbf{n}! = n_1! \cdots n_d!.$$

■

We turn now to the operators which satisfy the canonical commutation rules. These operators are known as the raising and lowering operators, or sometimes as the creation and annihilation operators. This latter name is better reserved for the field theoretic setting.

It is sufficiently general to define the raising and lowering operators as linear operators on a locally convex space. This next definition is basic for everything that follows, as it contains that class of *ccr* representations which is determined by the physics.

The basic mathematical structure associated with the canonical commutation relations, elaborated in this chapter, seems to have been enunciated first by Kristensen, Mejlbo, and Thue-Poulsen [1] in 1965. Our concerns here are slightly different from theirs, and we concentrate only on those representations of greatest physical interest. We have termed these s–class representations. After Proposition [2.25] we shall justify this choice in terms of the basic measurement principle noted in the preface: every observable shall be measurable in every state. By $E[t]$ we shall mean a complex vector space E with a locally convex topology t.

Definition 2.3 (a) Let Σ_d be an elementary quantum system with d degrees of freedom, neglecting spin. By a representation of the canonical commutation relations, or *ccr*, on an *lcs* $E[t]$ we mean

(i) an *lcs* space $E[t]$ with a continuous sesquilinear form $\langle \cdot, \cdot \rangle$ with respect to which E is a complex pre-Hilbert space, and

(ii) a family $\left(b_j, b_j^+\right)_{1 \leq j \leq d}$ of continuous linear operators on $E[t]$ which are adjoint with respect to the sesquilinear form $\langle \cdot, \cdot \rangle$, and satisfy

$$\left(b_j b_k^+ - b_k^+ b_j\right) u = \delta_{jk} u, \tag{2.1.a}$$

$$\left(b_j b_k - b_k b_j\right) u = 0, \tag{2.1.b}$$

and

$$\left(b_j^+ b_k^+ - b_k^+ b_j^+\right) u = 0, \tag{2.1.c}$$

for all $u \in E$ and all $1 \leq j, k \leq d$.

(b) The representation is said to be cyclic if there exists a non-zero vector $w \in E$ such that $\mathcal{P}w$ is dense in $E[t]$, where $\mathcal{P}$ is the algebra of all polynomials in the family $\left(b_j, b_j^+\right)_{1 \leq j \leq d}$. The vector w is then known as a cyclic vector. There is no loss of generality in assuming that w is normalized with respect to the inner product, and we do so: $\langle w, w \rangle = 1$.

(c) The representation is said to be s–class if it is cyclic and if the cyclic vector w satisfies the Fock condition

$$b_j w = 0, \qquad 1 \leq j \leq d, \tag{2.2}$$

and is the only normalized vector to do so. In such a case we refer to w as the Fock vector.

Let us agree to write

$$(\mathbf{b}, \mathbf{b}^+, E[t], w)$$

for an s–class representation, where $\mathbf{b}$ is vector notation for the operator valued d-tuple $b_1, \ldots, b_d$, and similarly for $\mathbf{b}^+$.

If the carrier space $E[t]$ is complete, then we say that we have a complete s–class representation. ■

In the last chapter, we stated that an s–class representation required a gauge invariant state. We also wrote down an expression for the gauge group operator Γ in equation (1.4). In Section 2.7 we shall identify the coordinate and momentum operators in terms of the raising and lowering operators. When we do, it will be seen that the generator of Γ can be written as $\overline{\sum b_j^+ b_j}$. Granting this, equation (2.2) shows that w is a gauge invariant vector. As vectors will be seen to determine states, this definition is consistent with our previous discussion.

It is known that representations of an algebra with an involution, such as $\mathcal{P}$, can behave badly with respect to involution. This has been analysed by Powers [1] and Gudder and Scruggs [1]. Conditions (a) and (b) above guarantee that no such pathologies occur for s–class representations. If we consider the completion of E with respect to the posited continuous inner product, the result is a rigged Hilbert space structure (Gel'fand and Vilenkin [1]). Ultimately, the origin of this requirement is that the basic physical observables be measurable, and their measurements yield real numbers. Thus, this is a physically motivated restriction.

It may seem a spurious generality to consider locally convex spaces rather than Hilbert spaces. As noted in the Introduction, so far from being the case, it is an absolute necessity, as at least one of the raising and lowering operators in each pair must be unbounded. For simplicity let us consider one pair only, $d = 1$. Suppose we assume a representation of the *ccr* on a Hilbert space. The requirement that b and b^+ be continuous is equivalent to their being bounded. It follows that $\mathcal{P}$ is a normed algebra with an identity. However, the Winter–Wielandt theorem precludes this, cf, Putnam [1].

2.4 Theorem There exists no Hilbert space $\mathcal{H}$ such that we can find continuous linear operators x, y on $\mathcal{H}$ satisfying the commutation relation $xy - yx = I$.

Proof Assume the contrary, from which it follows that for all $n \in \mathbb{N}$ we have the identity

$$xy^{n+1} - y^{n+1}x = (n+1)y^n.$$

Taking the operator norm of both sides leads to

$$(n+1)\,\|y^n\| \leq 2\,\|x\|\,\|y\|\,\|y^n\|,$$

and so $y^n = 0$ for large enough n. It follows from this and the first equation that $y^{n-1} = 0$. Downward induction leads to $y^0 = I = 0$, which is a contradiction. ■

The conditions defining an s–class representation of the *ccr* are patterned after the natural representation on $L^2\left(\mathbb{R}^d\right)$, the Schrödinger representation. It turns out that, up to isomorphism, this is the only complete s–class representation. In order to prove this we must first introduce some appropriate definitions and constructions.

2.4 RAPIDLY DECREASING SEQUENCES

The first definition is of the spaces of rapidly decreasing sequences and sequences which terminate. Over and above their intrinsic interest in the theory of topological vector spaces, they are important for *ccr* representations. As we shall later show, all s–class representations lie between them, up to isomorphisms.

2.5 Definition (a) By a rapidly decreasing sequence we mean a complex sequence

$$\mathbf{c} = (c_{\mathbf{n}})_{\mathbf{n}\in\mathbb{N}^d}$$

for which the sums

$$\|\mathbf{c}\|_r^2 = \sum\nolimits_{\mathbf{n}\in\mathbb{N}^d} (d + |\mathbf{n}|)^r |c_{\mathbf{n}}|^2 \tag{2.3}$$

converge, all $r \in \mathbb{N}$. It is evident from this that $\|\cdot\|_r$ is a norm.

By the space $s^{(d)}$ we mean the *lcs* of all rapidly decreasing sequences equipped with the topology ν determined by the seminorms $(\|\cdot\|_r)_{r\in\mathbb{N}}$.

(b) By a terminating sequence we mean a complex sequence $\mathbf{c} = (c_{\mathbf{n}})_{\mathbf{n}\in\mathbb{N}^d}$ for which only a finite number of coordinates $c_{\mathbf{n}}$ are nonzero.

By $\phi^{(d)}$ we shall mean the complex vector space of all terminating sequences. By $\phi^{(d)}[\nu]$ we mean $\phi^{(d)}$ equipped with the topology ν of $s^{(d)}$. ■

In Proposition [2.8] below, we shall show that the space of terminating sequences is dense in the space of rapidly decreasing sequences. The basic reference for sequence spaces is Köthe [1].

The reader will recall that the Hermite functions are solutions of one of the classical second order differential equations. In his researches on Fourier series, Wiener [1] made extensive use of the fact that the Hermite polynomials multiplied by the Gaussian constitute an orthonormal basis for $L^2(\mathbb{R}^3)$.

Quantum mechanics reintroduced these functions into Physics as the eigenfunctions of the simple harmonic oscillator Hamiltonian. It was a close analysis of the action of the position and momentum operators on these eigenfunctions that led to the discovery of the raising and lowering operators.

Subsequently it was discovered that these eigenfunctions constitute a Schauder basis (Jarchow [1]) for the Schwartz space of smooth functions of rapid decrease (Trèves [1]). We shall observe that this arises from the action of the raising and lowering operators. Moreover, this action has a counterpart in all *lcs* spaces carrying a *ccr* representation. As the Schwartz space is a universal generator for nuclear spaces (Kōmura's theorem, [2.22] below), we conclude that there is a deep connection between representations of the *ccr* and the category of nuclear *lcs* spaces. We emphasize this by starting our analysis of $s^{(d)}$ by means of the *ccr* . This approach, relating the Schwartz sequence space to the commutation relations, is due to Simon [1].

2.6 Definition (a) Let $(\mathrm{b}, \mathrm{b}^+, E[t], w)$ be an s–class representation of the *ccr* . The Hermite vectors are defined to be

$$w_{\mathbf{n}} = (\mathbf{n}!)^{-1/2}\mathrm{b}^{+\mathbf{n}} w_0, \qquad \mathbf{n} \in \mathbb{N}^d, \tag{2.4}$$

where we use multi-index notation, and have set $w = w_0$.

(b) We shall write

$$M_j = b_j b_j^+, \tag{2.5.a}$$

and

$$M = M_1 + \cdots + M_d. \tag{2.5.b}$$

By an inexact analogy with quantum field theory we refer to these operators as number operators; in particular, to M as the total number operator if a distinction is necessary. ■

We shall see below that in $L^2(\mathbb{R}^3)$ the above Hermite vectors constitute precisely the Hermite Schauder basis mentioned above.

Continuing our constructions, from equations (2.1) and (2.4), one can verify the following formulae for the Hermite vectors sufficiently easily so that we omit a proof. We re-emphasize that the connection between the *ccr* and nuclearity hinges on this lemma.

2.7 Lemma The raising and lowering operators act on the Hermite vectors of E as follows:

$$b_j w_{\mathbf{n}} = \sqrt{n_j}\, w_{(\dots,n_j-1,\dots)} \tag{2.6.a}$$

and

$$b_j^{\dagger} w_{\mathbf{n}} = \sqrt{n_j+1}\, w_{(\dots,n_j+1,\dots)}. \tag{2.6.b}$$

The Hermite elements are orthonormal with respect to the inner product on $E[t]$:

$$\langle w_{\mathbf{n}}, w_{\mathbf{m}} \rangle = \delta_{\mathbf{n},\mathbf{m}}, \tag{2.7}$$

with an obvious notation for the multi-indexed Kronecker delta. ■

The next results connect the spaces $\phi^{(d)}[\nu]$ and $s^{(d)}[\nu]$ as indicated above, and shows them to carry s–class representations of the *ccr* .

2.8 Proposition (a) $s^{(d)}[\nu]$ is the *tvs* completion of $\phi^{(d)}[\nu]$, hence a Fréchet space.

(b) The spaces $\phi^{(d)}[\nu]$ and $s^{(d)}[\nu]$ carry s–class representations of the *ccr* , and so the representation on $s^{(d)}[\nu]$ extends that on $\phi^{(d)}[\nu]$ and is complete.

(c) The Hermite vectors constitute a Schauder basis for $\phi^{(d)}[\nu]$ and $s^{(d)}[\nu]$, as well as being an orthonormal basis for the Hilbert space l_d^2 of square summable sequences from $\mathbb{N}^d$.

(d) Recalling the definition of the seminorms for the topology ν, the inner product on both spaces is just the usual Euclidean one, corresponding to $\|\cdot\|_0$:

$$\langle \mathbf{c}, \mathbf{c}' \rangle = \sum\nolimits_{\mathbf{n}\in\mathbb{N}^d} \overline{c_{\mathbf{n}}} c'_{\mathbf{n}}. \tag{2.8}$$

Thus $\phi^{(d)}[\nu]$ and $s^{(d)}[\nu]$ are continuously and densely embedded in l_d^2.

(e) In both cases the cyclic Fock vector is the sequence

$$(w_{\mathbf{0}})_{\mathbf{n}} = \delta_{\mathbf{0},\mathbf{n}}, \qquad \mathbf{0} = (0,\dots,0), \mathbf{n} \in \mathbb{N}^d. \tag{2.9}$$

(f) The raising and lowering operators on $\phi^{(d)}$ and $s^{(d)}$ are defined through formulæ obtained from equation (2.6) :

$$\left[b_j^+ \mathbf{c}\right]_{\mathbf{n}} = \sqrt{n_j}\, c_{(\ldots,n_j-1,\ldots)}, \tag{2.10.a}$$

and

$$\left[b_j \mathbf{c}\right]_{\mathbf{n}} = \sqrt{n_j+1}\, c_{(\ldots,n_j+1,\ldots)}. \tag{2.10.b}$$

Proof It is evident by direct calculation that the operators defined in equation (2.10) are raising and lowering operators satisfying the ccr . It is also immediate that w_0 is a Fock vector. It is also clearly the only such vector. This is easy to see for one degree of freedom. Given $\mathbf{c} \in l^2$, the equation $b\mathbf{c} = 0$ has the one point solution set $\{ c_0\, w_0 \}$.

Let us show that w_0 is cyclic for $\phi^{(d)}$. The essentials are clarified if we consider only one degree of freedom for a moment. By applying the raising operator b^+ successively, starting with equation (2.9) , the Hermite vector w_k is seen to be the sequence consisting of zeros except for unity in the k-th place. This family of sequences is well known to be a linear basis for $\phi^{(1)}$, all sums being finite.

For general d the procedure is evidently similar and leads to the formula

$$(w_{\mathbf{n}})_{\mathbf{m}} = \delta_{\mathbf{n},\mathbf{m}} \tag{2.11}$$

for the Hermite vectors. For any $\mathbf{c} \in \phi^{(d)}$,then, we have the unique finite expansion

$$\mathbf{c} = \sum c_{\mathbf{n}} w_{\mathbf{n}}. \tag{2.12}$$

As a finite sum, this expansion converges in the ν–topology, and we conclude that the Hermite vectors are a Schauder basis for $\phi^{(d)}[\nu]$ and w_0 is cyclic.

Turning to $s^{(d)}[\nu]$ next, for any $\mathbf{c} \in s^{(d)}$ we introduce the truncations $\mathbf{c}^i$, where $i \in \mathbb{N}$, obtained by setting to zero all components of $\mathbf{c}$ with $|\mathbf{n}| > i$. Elementary convergence theory for series gives us that $\mathbf{c}^i$ converges to $\mathbf{c}$ in the ν-topology, *ie* ,

$$\left\|\mathbf{c}^i - \mathbf{c}\right\|_r^2 = \sum\nolimits_{|\mathbf{n}|>i} (|\mathbf{n}| + d)^r \left|c_{\mathbf{n}}\right|^2 \tag{2.13}$$

converges to zero as $i \to \infty$.

Now expand $\mathbf{c}^i$ in terms of Hermite vectors as in equation (2.12) and insert into equation (2.13). This shows that every vector in $s^{(d)}[\nu]$ may be represented in terms of a ν–convergent series of Hermite vectors. The uniqueness of the expansion coefficients follows from the simple observation that $\|\cdot\|$ is a norm. Hence the Hermite vectors are a Schauder basis for $s^{(d)}[\nu]$. This also shows that $\phi^{(d)}[\nu]$ is dense in $s^{(d)}[\nu]$, and so w_0 is cyclic in $s^{(d)}[\nu]$.

That the Hermite vectors constitute a Hilbert basis for l^2_d is proved by the above argument, setting $\mathbf{c} \in l^2_d$ and $r = 0$.

As ν is determined by a countable family of seminorms, both $\phi^{(d)}[\nu]$ and $s^{(d)}[\nu]$ are metrizable. There are several ways to show that $s^{(d)}[\nu]$ is complete, *eg* , using the theory of sequence spaces. Another method will be given in the next section.

Now consider the continuity of the raising and lowering operators. Recalling the definition of the number operators, equation (2.5) , observe that with equation (2.12) , the ν–seminorms can be written as

$$\|\mathbf{c}\|_r^2 = \langle \mathbf{c}, M^r \mathbf{c}\rangle. \tag{2.14}$$

Note that this holds for both $\phi^{(d)}$ and $s^{(d)}$, in view of the above remarks.

Combining this with the identities

$$b_j M^r = (M+1)^r \, b_j \tag{2.15.a}$$

and

$$b_j^+ M^r = (M-1)^r \, b_j^+, \tag{2.15.b}$$

yields the equations

$$\sum\nolimits_{j \le d} \|b_j \mathbf{c}\|_r^2 = \langle \mathbf{c}, (M-1)^r (M-d)\, \mathbf{c}\rangle \tag{2.16.a}$$

and

$$\sum\nolimits_{j \le d} \left\|b_j^+ \mathbf{c}\right\|_r^2 = \langle \mathbf{c}, (M+1)^r M\mathbf{c}\rangle. \tag{2.16.b}$$

The continuity of the raising and lowering operators on both spaces is now immediate. We have now verified all the statements of the proposition. ∎

2.5 TOPOLOGICAL STRUCTURE OF $s^{(d)}$

As $s^{(d)}$ is so central to our considerations, it is useful to have as complete a characterization of it as possible. We shall prove below that in a certain sense it is completely determined by the number operator. In view of the definition of the seminorms of the ν-topology, that is not particularly surprising. As a first step in this characterization we consider the number operators as Hilbert space operators, and find that they have a rather simple character.

2.9 Lemma Let $E_{\mathbf{n}}$ be the projection operator on l_d^2 defined by extension from its action on the Hermite vectors, so that

$$E_{\mathbf{n}} w_{\mathbf{m}} = \delta_{\mathbf{n},\mathbf{m}} w_{\mathbf{n}}. \tag{2.17}$$

Then

$$\overline{M} = \sum_{\mathbf{n} \in \mathbb{N}^d} (|\mathbf{n}| + d) E_{\mathbf{n}} \tag{2.18}$$

is the spectral representation of the Friedrich's extension of the number operator M. It is self adjoint and has the discrete spectrum

$$\{\, |\mathbf{n}| + d : \mathbf{n} \in \mathbb{N}^d \,\}$$

of isolated eigenvalues; hence $\overline{M} \geq dI$. The eigenvalue $d + k$ of $\overline{M}$ has multiplicity given by the binomial coefficient C_{d-1}^{k+d-1}, and the corresponding eigenspace has the orthonormal basis

$$\{\, w_{\mathbf{n}} : |\mathbf{n}| = k \,\}.$$

By definition (Kato [1],VI.2.3; Reed and Simon [1]), the Friedrich's extension $\overline{M}$ is the operator associated with the form

$$\mathrm{t}[\mathbf{c}, \mathbf{d}] = \sum_{j \geq 0} (j + 1) \overline{c_j} d_j, \tag{2.19.a}$$

on the form domain

$$D(\mathrm{t}) = \left\{ \mathbf{c} \in s^{(1)} : \mathrm{t}[\mathbf{c}, \mathbf{c}] < \infty \right\}. \tag{2.19.b}$$

Each of the "mode" number operators M_j has a Friedrich's extension

$$\overline{M_j} = \sum_{k \geq 0} (k + 1) E_k^{(j)}. \tag{2.20.a}$$

The indicated spectral projection operators are given by

$$E_k^{(j)} = \sum_{\mathbf{n} \in \mathbb{N}^d} \delta_{k, n_j} E_{\mathbf{n}}. \tag{2.20.b}$$

Proof The only non-trivial part of the proof is that the form defined above, clearly an extension of the form defined by M on $s^{(d)}$, is symmetric, closed, and bounded below. From its definition we see that the form is symmetric and bounded below, with bound

$$\mathrm{t}[\mathbf{c}, \mathbf{c}] \geq d \|\mathbf{c}\|^2.$$

As the lower bound is d, by a well known theorem the form will be closed iff the form domain is complete in the norm $\mathrm{t}[\mathbf{c}, \mathbf{c}]^{1/2}$ (Reed and Simon [2], VIII.6). This completeness is shown in the same way as one shows that l_d^2 is complete, and so we omit it. We can conclude from this that the form represents the self adjoint operator which we have denoted $\overline{M}$, evidently an extension of M. The proof of the analogous statements for the M_j proceeds in the same way. ■

If the reader is not familiar with the relation between the *ccr* and $s^{(d)}$, it is an instructive exercise to consider the case $d = 2$ and arrange the components of sequences $\mathbf{c} \in s^{(2)}$ as infinite square matrices. The raising and lowering operators and the number operators can then be exhibited explicitly.

There are a number of natural ways to construct topologies on $s^{(d)}$. We have just considered one: using the number operator to define the ν-topology. This connects $s^{(d)}$ with the *ccr* .

A second topology to consider on $s^{(d)}$ arises from the rapid decrease of the sequences. Given any rapidly decreasing sequence $\mathbf{c}$, define the seminorms

$$\mathbf{c} \to \|\mathbf{c}\|_{\infty;r} = \sup\left\{ (|\mathbf{n}| + d)^r |c_{\mathbf{n}}| : \mathbf{n} \in \mathbb{N}^d \right\}, \tag{2.21}$$

for all $r \in \mathbb{N}$. Let us denote this topology ν_∞.

The third method is a special case of a general construction, which we now describe.

2.10 Definition Given a set $\mathcal{F}$ of operators containing the identity, acting on a normed space E, we consider the family

$$u \to \|u\|_a = \|au\|, \tag{2.22}$$

for all $a \in \mathcal{F}$ and all $u \in E$. These are seminorms and the family of them define the graph topology on E determined by $\mathcal{F}$, which we shall denote $\gamma_{\mathcal{F}}$. This is the coarsest locally convex topology on E for which all the operators of $\mathcal{F}$ and the norm are continuous. ■

With this notation we may consider the graph topology on $s^{(d)}$ determined by the algebra $\mathcal{P}$ of polynomials in the raising and lowering operators. The connection between the three topologies on $s^{(d)}$ just described is the content of the next proposition.

2.11 Proposition The three topologies on $s^{(d)}$ are mutually equivalent,

$$\nu \equiv \nu_\infty \equiv \gamma_{\mathcal{P}}. \tag{2.23}$$

Proof Let us make our usual simplification of taking one degree of freedom, $d = 1$, in the proof. It is evident that

$$\|\mathbf{c}\|_\infty \le \|\mathbf{c}\|_2$$

for all $\mathbf{c} \in l^2$.

Taking $c_n = (n+1)^r d_n$ for $r \in \mathbb{N}$ and $\mathbf{d} \in s^{(1)}$ in this last inequality gives the bound

$$\|\cdot\|_{\infty;r} \leq \|\cdot\|_{2;2r},$$

the latter being an occasional notation for the ν-norm $\|\cdot\|_{2r}$ so as to distinguish it from the l^2 norm.

It follows from the identity $c_n = (n+1)^{-1}(n+1)c_n$ that

$$\|\mathbf{c}\|_2 \leq \sqrt{\pi^2/6}\,\|\mathbf{c}\|_{\infty;1}.$$

The substitution $c_n = (n+1)^r d_n$, for $r \in \mathbb{N}$ and $\mathbf{d} \in s^{(1)}$, scales this up to

$$\|\mathbf{d}\|_{2;r} \leq \|\mathbf{d}\|_{2;2r} \leq \sqrt{\pi^2/6}\,\|\mathbf{d}\|_{\infty;r+1}.$$

With this we have shown that the topologies ν and ν_∞ are equivalent.

We shall show now that the graph topology is equivalent to ν. To start with, we have the equality

$$\|\mathbf{c}\|_r^2 = \begin{cases} \|M^s\mathbf{c}\|_0^2 & \text{if } r = 2s, \\ \sum_{j\leq d} \left\|b_j^\dagger M^s\mathbf{c}\right\|_0^2 & \text{if } r = 2s+1. \end{cases} \tag{2.24}$$

Note that we have returned to our earlier notation $\|\cdot\|_r$ for the ν-norms; the l^2 norm is then the case $r = 0$.

Equation (2.24) proves that the ν-norms are continuous for the graph topology. Referring back to equation (2.16) shows that the raising and lowering operators are continuous for the ν-topology. By repeated application of equation (2.15) we see that the same is true of any polynomial in the raising and lowering operators. Hence the graph seminorms are ν-continuous, and this completes the proof of the proposition.
■

A further analysis of the structure of $s^{(d)}$ requires the following lemma. This is the first step towards proving that $s^{(d)}$ is a countably Hilbert space.

2.12 Lemma (a) The seminorms defining the ν-topology are an increasing sequence of norms:

$$\|\mathbf{c}\|_{r-1}^2 \leq d^{-1}\|\mathbf{c}\|_r^2. \tag{2.25}$$

(b) The ν-norms are pairwise compatible: if a sequence $\mathbf{c}^i \in s^{(d)}$ is a Cauchy sequence for any two ν-norms and converges to zero in one of them, then it converges to zero for the other.

Proof That these seminorms are norms follows obviously from their definition. Equation (2.25) follows immediately from the useful identity

$$M = d + \sum_{j \le d} b_j^+ b_j .$$

Having shown these norms to be ordered, to prove compatibility it is sufficient to prove that if $\mathbf{c}^i$ converges to zero in the r-norm,

$$\left\| \mathbf{c}^i \right\|_r \to 0,$$

and is a Cauchy sequence for the $(r+1)$-norm, then it converges to zero in the $(r+1)$-norm.

As usual, we lose no real generality in proving this for one degree of freedom. Now as the sequence $\mathbf{c}^i$ is $(r+1)$-Cauchy, there is an element $\mathbf{d} \in l^2$ such that

$$l^2 - \lim_i \left([n+1]^{(r+1)/2} c_n^i \right)_{n \ge 0} = \mathbf{d}.$$

This implies that

$$\left\| \mathbf{c}^i - \left([n+1]^{-(r+1)/2} d_n \right)_{n \ge 0} \right\|_r \to 0.$$

But we know that $\left\| \mathbf{c}^i \right\|_r \to 0$. Hence

$$\left\| \left([n+1]^{-(r+1)/2} d_n \right)_{n \ge 0} \right\|_r = 0.$$

It is immediate that $\mathbf{d} = 0$ and we are done. ■

In Gel'fand and Shilov [1], it is shown that if $E[t]$ is a locally convex space, and if $\|\cdot\|_1$ and $\|\cdot\|_2$ are compatible continuous norms on E, such that

$$\|x\|_1 \le C \|x\|_2, \qquad C > 0, x \in E,$$

then the completions of E with respect to these norms are related by

$$E[t] \subset \overline{E[\|\cdot\|_1]} \subset \overline{E[\|\cdot\|_2]}.$$

This is now seen to hold for r-norms on $s^{(d)}$. Thus $s^{(d)}$ is a subset of the intersection of all the completions. We now show that it is equal to this intersection. But first we prove that we need only consider even indices.

2.13 Corollary Consider the family $(\|\cdot\|_r)_{r\geq 0}$ of norms defining the ν-topology, and its subfamily of even indexed norms $(\|\cdot\|_{2r})_{r\geq 0}$. Then every norm in the family is dominated by a norm in the subfamily and conversely.

Proof As we are considering a subfamily we need only show the domination of a norm with an odd index by one with an even index. But this is immediate from equation (2.25) . ■

We now prove the principal structure theorem for $s^{(d)}$, namely that it is a countably Hilbert space determined by the number operator M. In particular, equation (2.28) below shows that $s^{(d)}$ has an especially simple structure based on the ccr.

2.14 Theorem (a) Let $s_r^{(d)}$ be the completion of $s^{(d)}$ in the ν-norm $\|\cdot\|_{2r}$. Then each $s_r^{(d)}$ is a Hilbert space, and

$$s^{(d)} = \bigcap_{r\geq 0} s_r^{(d)}. \tag{2.26}$$

Equipped with the ν-topology, $s^{(d)}$ is a countably Hilbert space (Gel'fand and Vilenkin [1]).

(b) Let $\mathcal{P}(x_1, \ldots, x_n)$ be the $*$-algebra of all polynomials with complex coefficients in n free hermitian indeterminates. This algebra can be explicitly described in terms of monomials, and we refer the reader to, eg, Schmüdgen [2] for the construction. Let $A_1, \ldots, A_n$ be a family of operators on a Hilbert space $\mathcal{H}$. They need not commute nor be densely defined. The formal substitution of $A_1, \ldots, A_n$ for $x_1, \ldots, x_n$ results in the set we denote by $\mathcal{P}(A_1, \ldots, A_n)$. Writing $D(B)$ for the domain of an operator B, let us define

$$\mathcal{C}^\infty(A_1, \ldots, A_n) = \bigcap \{ D(B) : B \in \mathcal{P}(A_1, \ldots, A_n) \}. \tag{2.27.a}$$

For a single operator A we write

$$\mathcal{C}^\infty(A) = \bigcap_{r\geq 0} D(A^r). \tag{2.27.b}$$

The vectors in $\mathcal{C}^\infty(A_1, \ldots, A_n)$ are said to be smooth for the family $A_1, \ldots, A_n$.

Note that $\mathcal{C}^\infty(A_1, \ldots, A_n)$ may well be the singleton set $\{0\}$. Note also that $\mathcal{C}^\infty(A_1, \ldots, A_n)$ is stable under $\mathcal{P}(A_1, \ldots, A_n)$. In other words, an element of $\mathcal{P}(A_1, \ldots, A_n)$ may be regarded as an endomorphism of $\mathcal{C}^\infty(A_1, \ldots, A_n)$.

Then taking $A = \overline{M}$ and $\mathcal{H} = l_d^2$, we see that

$$s^{(d)} = \mathcal{C}^\infty(\overline{M}). \tag{2.28}$$

Proof We know that the ν-topology seminorms are norms, and we observe that the $2r$-norm may be obtained from the inner product

$$\langle \mathbf{c}, \mathbf{d} \rangle_r = \langle M^r \mathbf{c}, M^r \mathbf{d} \rangle \tag{2.29.a}$$

$$= \sum_{\mathbf{n} \in \mathbb{N}^d} (|\mathbf{n}| + d)^{2r} \overline{c_{\mathbf{n}}} d_{\mathbf{n}}. \tag{2.29.b}$$

It is therefore clear that

$$s_r^{(d)} = \left\{ \mathbf{c} : \sum_{\mathbf{n} \in \mathbb{N}^d} (|\mathbf{n}| + d)^{2r} |c_{\mathbf{n}}|^2 < \infty \right\}.$$

Equation (2.26) is now immediate.

Having established equation (2.26) , we wish to show that the ν-topology is countably normed. This requires that the defining norms be compatible; we have shown this in Lemma [2.12], thus completing the proof of (a).

The proof of (b) follows immediately from this by noticing that $s_r^{(d)}$ is the form domain of the Friedrich's extension of the operator $\overline{M^r}$. ■

The notation of equation (2.27) comes about as follows. Suppose we consider the particular case where the Hilbert space is $L^2(\mathbb{R}^d)$ and A_1, A_2, ..., A_d, are the operators of differentiation in each variable. Then (2.27) yields the space of infinitely differentiable functions.

For our purposes, we may extend this example by supplementing the derivative operators by the operators of multiplication by the coordinate functions; denote these as A_{d+1}, A_{d+2}, ..., A_{2d}. Now (2.27) yields Schwartz's space of infinitely differentiable functions of rapid decrease, $\mathcal{S}\left(\mathbb{R}^d\right)$. This will be shown to be isomorphic to $s^{(d)}$, a result which is important for the physical interpretation of the model. But first we proceed with our analysis.

It is now an easy matter to determine which class of topological vector space $s^{(d)}$ belongs to. We include a proof only because the nuclearity of $s^{(d)}$ is central to our theory.

2.15 Proposition The space $s^{(d)}[\nu]$ is a countably Hilbert nuclear Fréchet space. Hence it is barreled, bornological, Montel, reflexive and separable.

The triple

$$s^{(d)}[\nu] \subseteq l_d^2 \subseteq \left(s^{(d)}[\nu] \right)'_b$$

is a rigged Hilbert space. That is, the inclusions are continuous and have dense ranges.

Proof We need only prove that $s^{(d)}[\nu]$ is nuclear, as we have shown it to be countably Hilbert and Fréchet . As $s^{(d)}[\nu]$ is countably Hilbert, a necessary and sufficient condition for nuclearity is that for any r there is a $t > r$ such that the standard injective mapping

$$\iota_{tr} : s_t^{(d)} \longrightarrow s_r^{(d)}$$

is nuclear, cf, Gel'fand and Vilenkin [1], I.3.2.

For any $r \in \mathbb{N}$, the family

$$w_{\mathbf{n}}^r = (|\mathbf{n}| + d)^{-r/2}\, w_{\mathbf{n}}, \qquad \mathbf{n} \in \mathbb{N}^d$$

is an orthonormal basis for $s_r^{(d)}$. Then for $t > r + 2$,

$$\iota_{tr}(\xi) = \sum\nolimits_{\mathbf{n}} \langle w_{\mathbf{n}}^t, \xi\rangle_t\, (|\mathbf{n}| + d)^{(r-t)/2}\, w_{\mathbf{n}}^r, \qquad \xi \in s_t^{(d)}.$$

This shows that ι_{tr} is a nuclear map.

The remainder of the conditions of part (a) follow from the fact that $s^{(d)}[\nu]$ is a nuclear Fréchet space, and is standard *tvs* theory, cf, Bourbaki [1], Jarchow [1], Köthe [1], Robertson and Robertson [1], Schaeffer [1], Trèves [1], Wilansky [1].

Regarding the rigged triple property, we know that $s_0^{(d)}$ is just l_d^2, and so $s^{(d)}$ is dense and continuously embedded in l_d^2. This proves the existence of a continuous injection with dense range,

$$T : s^{(d)}[\nu] \rightarrow l_d^2.$$

The transpose, T', maps l_d^2 continuously into $s^{(d)}[\nu]'$, as l_d^2 is self dual.

As T is injective, T' has range which is dense in the Mackey topology. Since $s^{(d)}[\nu]$ is reflexive, the strong dual topology equals the Mackey topology. Because T has dense range, T' is injective. ■

We note in passing that the above representation of $s^{(d)}$ as a countably Hilbert space yields another proof of its completeness.

Our final topic in the analysis of $s^{(d)}$ in this section concerns its bounded subsets. By definition, a subset $B \subseteq s^{(d)}[\nu]$ is bounded if and only if for each index r there is a positive constant C_r, depending upon r and B, such that

$$\|\mathbf{c}\|_r \leq C_r, \qquad \mathbf{c} \in B.$$

We also recall that a family $\mathtt{B}$ of bounded subsets is said to be total if for any bounded subset F, there is a $B \in \mathtt{B}$ such that $F \subseteq B$. The explicit characterization of the bounded subsets of spaces of the form $\mathcal{C}^\infty(A)$ is due to Lassner [5].

2.16 Proposition Let a bijective set map $\kappa : \mathbb{N}^d \to \mathbb{N}$ be chosen. This determines an order on $\mathbb{N}^d$ by setting $\mathbf{n} \preceq \mathbf{m}$ if and only if $\kappa(\mathbf{n}) \leq \kappa(\mathbf{m})$. Without loss of generality, we choose κ such that

$$|\mathbf{n}| < |\mathbf{m}| \qquad \Longrightarrow \qquad \kappa(\mathbf{n}) < \kappa(\mathbf{m}).$$

Let Γ be the subset of $s^{(d)}$ consisting of all ordered positive sequences. By positive we mean that $v_{\mathbf{n}} \geq 0$ for all indices $\mathbf{n}$, and the ordering is obtained from the index order above. Thus

$$v_{\mathbf{n}} \geq v_{\mathbf{m}} \qquad \text{if and only if} \qquad \mathbf{n} \preceq \mathbf{m}.$$

Then for each $\mathbf{v} \in \Gamma$, the set of sequences

$$B_{\mathbf{v}} = \{\, (z_{\mathbf{n}} v_{\mathbf{n}}) : |z_{\mathbf{n}}| \leq 1 \,\} \tag{2.30.a}$$

is a bounded subset of $s^{(d)}[\nu]$; and

$$\mathrm{B}_\Gamma = \{\, B_{\mathbf{v}} : \mathbf{v} \in \Gamma \,\} \tag{2.30.b}$$

is a total family.

Proof We start by showing that the set $B_{\mathbf{v}}$ is bounded. For any $\mathbf{c} \in B_{\mathbf{v}}$ we have

$$\begin{aligned}
\|\mathbf{c}\|_{2r}^2 &= \sum |c_{\mathbf{n}}|^2 (|\mathbf{n}| + d)^{2r} \\
&= \sum |v_{\mathbf{n}}|^2 |z_{\mathbf{n}}|^2 (|\mathbf{n}| + d)^{2r} \\
&\leq \|\mathbf{v}\|_{2r}^2 .
\end{aligned}$$

As $\mathbf{v}$ is an element of $s^{(d)}$, the supremum over all $\mathbf{c} \in B_{\mathbf{v}}$ in this expression is finite, which proves the first half of the proposition.

Next we start with an arbitrary bounded subset V of $s^{(d)}$. We use V to construct a certain element $\mathbf{v} \in \Gamma$, and show that $V \subseteq B_{\mathbf{v}}$; this will prove that B_Γ is a total family of bounded subsets. The definition of $\mathbf{v}$ proceeds in two steps. First we define an auxiliary sequence $\mathbf{u}$ by choosing its components to be

$$u_{\mathbf{n}} = \sup\{\, |c_{\mathbf{n}}| : \mathbf{c} \in V \,\};$$

the second step is to set

$$v_{\mathbf{n}} = \sum\nolimits_{\mathbf{m} \succeq \mathbf{n}} u_{\mathbf{m}}.$$

Let us show that $\mathbf{v}$ is an element of Γ. That it is ordered and positive is obvious, so we consider its fall-off properties.

Now

$$(|\mathbf{n}|+d)^r|v_{\mathbf{n}}| \le \sum_{\mathbf{m}\succeq\mathbf{n}}(|\mathbf{m}|+d)^r \sup_{\mathbf{c}\in V}|c_{\mathbf{m}}|$$
$$\le C\,\sup_{\mathbf{c}\in V}\left[\sup_{\mathbf{k}\in\mathbb{N}^d}(|\mathbf{k}|+d)^{r+2}|c_{\mathbf{k}}|\right]$$
$$= C\,\sup_{\mathbf{c}\in V}\|c\|_{\infty;r+2}.$$

The constant C is given by

$$C=\sum_{\mathbf{n}\in\mathbb{N}^d}(|\mathbf{n}|+d)^{-2}.$$

Thus $\|v\|_{\infty;r}$ is finite for all $r\ge 0$; hence $\mathbf{v}\in\Gamma$.

Now let $\mathbf{c}\in V$ be arbitrary, and use it to define

$$z_{\mathbf{n}}=c_{\mathbf{n}}/v_{\mathbf{n}}.$$

Clearly $\mathbf{z}$ satisfies the inequality

$$|z_{\mathbf{n}}|\le 1.$$

As $v_{\mathbf{n}}\in\Gamma$, the identity

$$c_{\mathbf{n}}=z_{\mathbf{n}}v_{\mathbf{n}}$$

proves that $\mathbf{c}\in B_{\mathbf{v}}$ and the proof of the proposition is complete. ■

The structure of the sets in B_Γ is surprisingly simple and explicit. The only complication comes from having to provide an order for the multi–indices. This ordering problem will recur when we compound systems. This ends our analysis of $s^{(d)}$ for the present.

2.6 UNIQUENESS OF s–CLASS REPRESENTATIONS

We now know that both $\phi^{(d)}$ and $s^{(d)}$ carry s–class representations of the *ccr* when equipped with the ν-topology; that the ν completion of $\phi^{(d)}$ is $s^{(d)}$; and that the extension of the $\phi^{(d)}$ *ccr* representation to $s^{(d)}$ coincides with the original representation carried by $s^{(d)}$. It will turn out that the representation carried by $\phi^{(d)}$ is the smallest, and that on $s^{(d)}$ the largest, in a sense to be made precise. The material in this section is an elaboration of the uniqueness theorem of Kristensen, Mejlbo, and Thue-Poulsen [1].

There is another topology on $\phi^{(d)}$ which will be of some interest in this regard.

2.17 Proposition The space $\phi^{(d)}$ may be represented as an algebraic direct sum

$$\phi^{(d)}=\sum^{\oplus}_{\mathbf{n}\in\mathbb{N}^d}\mathbb{C}_{\mathbf{n}}, \tag{2.31.a}$$

where each $\mathbb{C}_{\mathbf{n}}$ is defined to be a copy of $\mathbb{C}$. By λ we mean the locally convex direct sum topology on $\phi^{(d)}$ associated with this realisation. The seminorms defining this topology are

$$p_{\mathbf{a}}(\mathbf{c}) = \sum_{\mathbf{n}\in\mathbb{N}^d} a_{\mathbf{n}}|c_{\mathbf{n}}|, \tag{2.31.b}$$

as a varies over all positive sequences. That is, sequences with positive components but no convergence constraints.

Then $\phi^{(d)}[\lambda]$ carries an s–class representation of the *ccr* . We omit the proof, noting only that the action of the raising and lowering operators on the c may be transferred to the a without affecting positivity. This will prove continuity, and the rest is obvious. ■

We remind the reader that (2.31.a) has the consequence that the correspondence (take $d = 1$)

$$(c_0, c_1, \ldots, c_n, 0, \ldots) \to c_0 + c_1 X + \cdots + c_n X^n$$

affords an isomorphism between ϕ as a symmetric tensor algebra, and the algebra of polynomials in one indeterminate, X, Greub [1]. We shall not use this observation, but we remark that it points the way to a space free formulation of the model.

Now consider an arbitrary s–class representation of the *ccr* on $E[t]$. We now prove that $\phi^{(d)}$ can be identified with the smallest subspace of $E[t]$ carrying an s–class representation.

2.18 Lemma Let E_m be the linear subspace of E spanned by the Hermite vectors. The map

$$J : \phi^{(d)} \to E_m,$$

obtained by linear extension from the identification of Hermite vectors, is a linear isomorphism.

Using J let us transfer the two topologies ν and λ to E_m, as well as restricting the given topology t. On E_m we have

$$\nu \preceq t \preceq \lambda.$$

Equipped with each of these topologies, E_m carries an s–class representation of the *ccr*

Proof As the Hermite vectors constitute an orthonormal basis for $\phi^{(d)}$and E_m as pre-Hilbert spaces, and only finite sums are involved, the linear isomorphism is clear.

The intertwining relations follow immediately from the definition of the Hermite vectors. Hence $E_m[\lambda]$ carries an s–class representation.

Each subspace $\mathbb{C}_n$ is spanned by a Hermite vector, and λ is the finest topology for which the injections $\mathbb{C}_n \to \phi^{(d)}$ are continuous. Thus $J : \phi^{(d)}[\lambda] \to E[t]$ is continuous, and so $t \preceq \lambda$. But the raising and lowering operators on $E_m[t]$ are continuous, as it carries an s–class representation, so $\nu \preceq t$.

The ν-topology is equivalent to the graph topology, and the graph topology is constructed so as to be the coarsest locally convex topology on $\phi^{(d)}$ for which the polynomials in the raising and lowering operators are continuous. ■

Gathering together all the strands, we can now state the basic uniqueness theorem for *ccr* representations.

2.19 Theorem Let $E[t]$ be any s–class representation of the *ccr* . There exist minimal and maximal s–class representations $E_m[\lambda]$ and $E_M[\nu]$ such that

$$E_m[\lambda] \hookrightarrow E[t] \hookrightarrow E_M[\nu]. \tag{2.32.a}$$

The $\hookrightarrow$ is meant both as dense continuous injections of topological vector spaces, and as continuous extensions of the polynomial algebra of the raising and lowering operators, with Fock vectors identified.

In the same double sense the minimal and maximal representations are equivalent to

$$E_m[\lambda] \cong \phi^{(d)}[\lambda], \tag{2.32.b}$$

and

$$E_M[\nu] \cong s^{(d)}[\nu]. \tag{2.32.c}$$

The maximal space can therefore be represented as a countably Hilbert nuclear Fréchet space

$$E_M[\nu] = \bigcap_{r \geq 0} E_M^{(r)}, \tag{2.33}$$

where $E_M^{(r)}$ is the completion of E_M in the ν-norm

$$u \to \|u\|_{2r} = \left\| \overline{M}^r u \right\|_0. \tag{2.34}$$

In this notation, $E_M^{(0)}$ is a Hilbert space, satisfying the isomorphism

$$E_M^{(0)} \cong l_d^2. \tag{2.35}$$

It follows that

$$E_M[\nu] \subseteq E_M^{(0)}[\, \|\cdot\|_0 \,] \subseteq E_M[\nu]'_b \tag{2.36}$$

is a rigged triple.

Along with equation (2.33) we have the representation

$$E_M[\nu] = \mathcal{C}^\infty\left(\overline{M}\right). \tag{2.37}$$

Proof The space $E_m[\lambda]$ is continuously and injectively embedded in $E_m[t]$, since $t \preceq \lambda$, and $E_m[t]$ is a dense subspace of $E[t]$, as the latter carries an s–class representation of the *ccr* . This establishes the first statement in equation (2.32.a).

Let $\mathcal{H}$ be the Hilbert space completion of $(E, \langle , \rangle)$. For any $\mathbf{n} \in \mathbb{N}^d$, let $g_\mathbf{n} : E \to \mathbb{C}$ be the linear functional defined by

$$g_\mathbf{n}(x) = \langle w_\mathbf{n}, x \rangle, \qquad x \in E.$$

Clearly, $g_\mathbf{n}$ is continuous on $(E, \langle , \rangle)$, and hence continuous on $E[t]$, the inner product being t-continuous.

By construction, $E_m[\nu] \cong \phi^{(d)}[\nu]$. Since $\phi^{(d)}$ is dense in $s^{(d)}[\nu]$, if we define $E_M[\nu]$ to be the completion of $E_m[\nu]$, it is clear that $E_M[\nu] \cong s^{(d)}[\nu]$. Let $f : E_M \to s^{(d)}$ implement this isomorphism.

Since $\nu \preceq t$, the identity map $\iota : E_m[t] \to E_m[\nu]$ is continuous and bijective. Thus it extends uniquely to a continuous linear map $\hat{\iota} : E[t] \to E_M[\nu]$. To complete the proof of the validity of equation (2.32) , it is now sufficient to show that $\hat{\iota}$ is injective.

Now for any $\mathbf{n} \in \mathbb{N}^d$, let us define the map $f_\mathbf{n} \in s^{(d)}[\nu]'$ by $f_\mathbf{n}(\mathbf{c}) = c_\mathbf{n}$. Then $f_\mathbf{n} \circ f \circ \hat{\iota} : E[t] \to \mathbb{C}$ is continuous and linear and coincides with $g_\mathbf{n}$ on E_m.

Then both $g_\mathbf{n}$ and $f_\mathbf{n} \circ f \circ \hat{\iota}$ are continuous extensions of $f_\mathbf{n} \circ f \circ \iota$ from E_m to E; hence they are equal. It follows that

$$f \circ \hat{\iota}(x) = \left(\langle w_\mathbf{n}, x \rangle\right)_\mathbf{n}, \qquad x \in E.$$

If $x \in E$ and $\hat{\iota}(x) = 0$, we deduce that $\langle w_\mathbf{n}, x \rangle = 0$ for all $\mathbf{n} \in \mathbb{N}^d$. Then

$$x = \sum\nolimits_\mathbf{n} \langle w_\mathbf{n}, x \rangle \, w_\mathbf{n} = 0$$

as an element of $\mathcal{H}$, hence in E. This proves that $\hat{\iota}$ is injective, and completes the proof. ■

Summarizing, any s–class representation of the *ccr* contains a copy of the representation on $\phi^{(d)}$ and is contained in a copy of the one on $s^{(d)}$, up to equivalence. This latter representation is the completion of any subrepresentation, and it is reasonable to say that it is maximal.

In the next section, we introduce the physically most natural representation, due to Schrödinger. This representation will be seen to be maximal, justifying the introduction of our notion of s–class.

Historically, the representation on $s^{(1)}$ was introduced by Heisenberg in the first paper on quantum mechanics [1]. The elucidation of Heisenberg's formalism is due to Born and Jordan [1], and Born, Jordan and Heisenberg [1]. In the physics literature, this representation goes under the name matrix mechanics.

So far we have considered only cyclic representations, those for which

$$\mathcal{P}w_0 = E_m$$

is dense in E. Suppose we extend the class of representations by relaxing the Fock condition, so that there can be more than one normalized vector which is annihilated by the lowering operators. We shall call these reducible representations.

2.20 Proposition Let there be given a representation of the *ccr* on the space $E[t]$ such that there is at least one Fock vector, but there can be countably many. Then there exist minimal and maximal *ccr* representations $E_m[\lambda]$ and $E_M[\nu]$ such that

$$E_m[\lambda] \hookrightarrow E[t] \hookrightarrow E_M[\nu]. \tag{2.38.a}$$

Just as for s–class representations, the ν- topology is determined by the norms

$$u \to \|u\|_{2r} = \left\|\overline{M}^r u\right\|_0. \tag{2.38.b}$$

Setting $E_M^{(0)}$ to be the completion of E_M in the ν-norm $\|\cdot\|_0$, it is a Hilbert space, and

$$E_M[\nu] \subseteq E_M^{(0)}[\|\cdot\|_0] \subseteq E_M[\nu]'_b \tag{2.38.c}$$

is a rigged triple.

The essential contrast to s–class representations is that $E_M^{(0)}$ reduces to a direct sum

$$E_M^{(0)} = \bigoplus \mathcal{H}^{(\alpha)}. \tag{2.39}$$

Along with this the triple of E, the minimum and the maximum spaces also reduce. In an obvious notation,we have the respective locally convex direct sums

$$E_m[\lambda] = \sum_\alpha^{\oplus} E_m^{(\alpha)}[\lambda^{(\alpha)}] \tag{2.40.a}$$

and

$$E_M[\nu] = \sum_\alpha^{\oplus} E_M^{(\alpha)}[\nu^{(\alpha)}]. \tag{2.40.b}$$

For each index α we get an s–class representation.

Proof The proof is an application of the spectral theorem to the self adjoint number operator and we refer the reader to Putnam [1], §4.4 for details. The principal idea in the proof is the following. One chooses an orthonormal basis $\left(w_0^{(\alpha)}\right)_\alpha$ for the closed Hilbert subspace of $E_M^{(0)}$ of all vectors satisfying $\overline{M}u = 0$. Just as for the case of s–class representations one can form the Hermite vectors from the raising operators acting on each $w_0^{(\alpha)}$, and for each α the analysis is the same as above. ∎

Remarks 2.21 (a) For contact with the natural world, a scale factor must be inserted in all of the above. This is Planck's constant, $\hbar = 1.0545 \times 10^{-27}$ erg sec. The scaling is explicitly given by

$$b_j^{\diamond} \to \sqrt{\hbar}\, b_j^{\diamond}, \tag{2.41}$$

and we shall assume this to have been done when appropriate. The superscript $^\diamond$ indicates that either the raising or the lowering operator is meant.

(b) The Fock condition is extremely restrictive, leading as it does to the above uniqueness theorem. Without this restriction there are uncountably many inequivalent representations of the *ccr* . The study of these representations involves many difficult technical problems. For a sample of these and back references, we suggest consulting the work of Schmüdgen [6,7]. Below, we shall give a simple example of a *ccr* representation which is neither s–class nor a direct sum of them. ∎

We have shown that $s^{(d)}$ can be constructed out of the *ccr* . It is doubly interesting, therefore, that $s^{(d)}$ is itself universal in the following sense.

2.22 Kōmura's Theorem An *lcs* is nuclear if and only if it is *tvs* -isomorphic to a subspace of the product space $s^{(I)}$ for some set I. A metrizable *lcs* is nuclear iff it is *tvs* -isomorphic to a subspace of $s^{(\mathbb{N})}$. For a proof see Jarchow [1], §21.7. ∎

2.7 THE SCHRÖDINGER REPRESENTATION

As is well known, the sequence space $s^{(d)}$ is isomorphic, as a topological vector space, to Schwartz's space of smooth functions of rapid decrease at infinity, $\mathcal{S}\left(\mathbb{R}^d\right)$. This isomorphism carries the s–class representation of the *ccr* on $s^{(d)}$ with it. The representation so obtained is of independent interest, and is the subject of this section. We shall see that the corresponding Hermite vectors are the functions originally studied by Hermite. Otherwise said, the Hermite differential equation is an eigenvalue equation for the total number operator in this representation.

We start by relating Schwartz's space to the number operator formalism.

2.23 Proposition Let

$$\mathcal{S}\left(\mathbb{R}^d\right) = \left\{ u \in C^\infty\left(\mathbb{R}^d\right) : \|u\|_{\mathbf{n},\mathbf{m}} < \infty,\ \mathbf{n},\mathbf{m} \in \mathbb{N}^d \right\}, \tag{2.42}$$

where

$$\|u\|_{\mathbf{n},\mathbf{m}} = \sup\left\{ |\mathbf{x}^{\mathbf{n}} \partial^{\mathbf{m}} u(\mathbf{x})| : \mathbf{x} \in \mathbb{R}^d \right\}. \tag{2.43}$$

By the usual topology on $\mathcal{S}\left(\mathbb{R}^d\right)$ we mean the topology determined by these semi-norms (Trèves [1], Gel'fand and Shilov [1]).

The raising and lowering operators are defined on $\mathcal{S}\left(\mathbb{R}^d\right)$ by

$$b_j = 2^{-1/2}\left(x_j + \partial/\partial x_j\right) \tag{2.44.a}$$

and

$$b_j^+ = 2^{-1/2}\left(x_j - \partial/\partial x_j\right). \tag{2.44.b}$$

The Fock vector is the Gaussian function

$$w_0(\mathbf{x}) = \pi^{-d/4} \exp\left(-\|\mathbf{x}\|^2/2\right). \tag{2.45}$$

If we define the Hermite vectors from the raising operators acting on this Gaussian, the resulting structure is an s–class representation of the *ccr* . Moreover, the ν-topology is equivalent to the usual topology, and $\mathcal{S}\left(\mathbb{R}^d\right)$ is a maximal space.

Proof It is clear that equation (2.44) defines operators that map $\mathcal{S}\left(\mathbb{R}^d\right)$ to itself and satisfy the *ccr* . Also clear is that the d-dimensional normalized Gaussian w_0 is an element of $\mathcal{S}\left(\mathbb{R}^d\right)$. Note that the Fock condition is a set of d differential equations of first order, whose solution space is one dimensional, spanned by w_0. Thus w_0 is a Fock vector.

We can apply our uniqueness theorem now, but this does not by itself relate the topologies. For this we must know that $\mathcal{S}\left(\mathbb{R}^d\right)$ is a Fréchet space in its usual topology. This is such a well known result that we shall simply assume it.

Were the topologies not equivalent, we could transfer the usual topology to the ν-completion $E_M[\nu]$ of $\mathcal{S}\left(\mathbb{R}^d\right)$, the maximal space of the uniqueness theorem. This would yield a Fréchet space with a second, strictly coarser separated metric topology, which is impossible by the closed graph theorem, cf, Robertson and Robertson [1], $VI.3$. ∎

The method of Fourier transformation is useful when considering differential operators. In general, Fourier transformation is a map between different spaces of test functions. However, for $\mathcal{S}\left(\mathbb{R}^d\right)$ it is an isomorphism. This will prove useful with regard to the Schrödinger representation. For a proof, cf, Trèves [1], Yosida [1].

2.24 Theorem Our convention for the Fourier transform on $\mathbb{R}^d$ is

$$\tilde{u}(\mathbf{k}) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} u(\mathbf{x}) \exp(i\mathbf{k}\cdot\mathbf{x})\, d\mathbf{x}, \tag{2.46.a}$$

and its inverse is

$$u(\mathbf{x}) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \tilde{u}(\mathbf{k}) \exp(-i\mathbf{k}\cdot\mathbf{x})\, d\mathbf{k}. \tag{2.46.b}$$

Writing

$$\tilde{u} = \mathcal{F}u \qquad \text{and} \qquad u = \mathcal{F}^{-1}\tilde{u}, \tag{2.46.c}$$

the map $\mathcal{F}$ is a unitary transformation on $L^2(\mathbb{R}^d)$ and a *tvs* isomorphism of $\mathcal{S}(\mathbb{R}^d)$ onto itself. ■

The representation of the *ccr* on $\mathcal{S}(\mathbb{R}^d)$ was, in essence, the one found by Schrödinger [1–4] in his papers on wave mechanics, hence the name Schrödinger representation. In these first papers the emphasis was on the position and momentum operators, which we shall now introduce. It is interesting to note that Schrödinger also introduced the raising and lowering operators on $\mathcal{S}(\mathbb{R}^1)$ as a factorisation method for solving the eigenvalue problem associated with the simple harmonic oscillator.

2.25 Proposition By the coordinate and momentum operators on $\mathcal{S}(\mathbb{R}^d)$ we mean the operators given by the formulas

$$[q_j u](\mathbf{x}) = x_j u(\mathbf{x}) \tag{2.47.a}$$

and

$$[p_j u](\mathbf{x}) = -i\,[\partial u/\partial x_j](\mathbf{x}), \tag{2.47.b}$$

respectively. As usual, $1 \le j \le d$. These operators are essentially self adjoint on $L^2(\mathbb{R}^d)$.

On the domain $\mathcal{S}(\mathbb{R}^d)$ they satisfy the *ccr* in the form

$$q_j p_k - p_k q_j = i\delta_{jk}, \tag{2.48.a}$$

$$q_j q_k - q_k q_j = 0, \tag{2.48.b}$$

and

$$p_j p_k - p_k p_j = 0, \tag{2.48.c}$$

where $1 \le j,k \le d$.

Along with equation (2.28) we have the important structural relation

$$\mathcal{S}(\mathbb{R}^d) = \mathcal{C}^\infty(q_1, p_1, \ldots, q_d, p_d). \tag{2.49}$$

Proof For simplicity, let us consider the case $d = 1$. The operator q will be shown to be essentially self adjoint if we can show that the range of the pair $q \pm i$ is dense.

Given $u \in \mathcal{S}\left(\mathbb{R}^1\right)$, define the function $v_\pm$ by

$$v_\pm(x) = (x \pm i)^{-1} u(x).$$

Using Leibnitz's rule for the derivative of a product, it is easy to verify that

$$\|v_\pm\|_{n,m} \leq \sum_{k=0}^{m} \binom{m+k}{k} \|u\|_{n,k},$$

as $|x \pm i|^{-1} \leq 1$. It follows from this that $v_\pm$ is an element of $\mathcal{S}\left(\mathbb{R}^1\right)$. Then the position operator is essentially self adjoint and $\mathcal{S}\left(\mathbb{R}^1\right)$ is a core for it.

For the momentum operator we use the above result concerning the Fourier transform. It is the characteristic property of the Fourier transform that it intertwines the position and momentum operators:

$$\mathcal{F} q = p \mathcal{F}, . \tag{2.50}$$

Now it is clear from this that the Fourier transform maps the range problem for $p \pm i$ to the range problem for $q \pm i$. It follows that the momentum operator is essentially self adjoint because the position operator is. The proof for general d is similar.

Regarding equation (2.49), comparison with equation (2.42) shows that it is precisely the original definition, now that the momenta have been identified as derivatives.

Finally, the *ccr* are an immediate consequence of the definitions and the stability of $\mathcal{S}\left(\mathbb{R}^d\right)$ under the operators. ■

Physical Scholium We have not as yet given any reason for referring to the above operators as position and momentum. Historically this identification is tied up with the wave mechanics of Schrödinger . Now Schrödinger's wave equation is obtained by combining Hamilton–Jacobi theory, which relates geometrical optics and particle dynamics (Arnold [1]), with de Broglie's hypothesis concerning the wave nature of matter (de Broglie [1-3]).

The similarity of this formalism to the Hamilton equations of classical mechanics is maximized by just this identification, which is then raised to the status of an axiom.

Reinforcement of this connection is obtained from the classical limit in two senses. Suppose we scale Planck's constant back into the theory, as indicated before. The right hand side of equations (2.47.b) and (2.48.a) will then be replaced by $i \rightarrow i\hbar$. As emphasized by Dirac, the quantum commutators approach the classical Poisson brackets in the limit $\hbar \to 0$. Here we may include the commutators of all allowable functions of the position and momentum operators. This is the first reinforcement.

Parenthetically, we note that the relation between commutators and Poisson brackets is not an equality, but a more complicated association, studied under the name geometric quantization. One formulation is to construct a deformation of the quantum algebra, determined by Planck's constant. The classical phase space functions are deformation equivalence classes of their quantum analogues. With this important proviso, we may understand the above statement (Lichnerowicz [1]).

The second is that there is an average sense in which the quantum mechanical operators obey classical equations of motion, due to Ehrenfest. We shall later show this, and it will follow that the time evolution of the position and momentum operators will approach the Hamilton equations of motion, again as $\hbar \to 0$

The above self adjointness result opens up an interesting possibility. We can use the position and momentum operators to generate unitary groups. These groups consist of bounded operators, and will lead to a C^*–algebra for the *ccr* . This exponentiation of the *ccr* is due to Weyl [1], IV.14. The results given below can be reversed logically, and then give another reason for the identification of the position and momentum operators as above. That is, they are the generators of the space and momentum translation groups. This corresponds to their identification as the generators of phase space translations in classical mechanics (Arnold [1]). We will discuss this in detail in [2.26-2.28] just below.

Granting this, we come to the justification for the introduction of s–class representations; it is essentially equation (2.49). We start from our measurement principle. This translates to the statement that wave functions must be the elements of $\mathcal{C}^\infty(q_1, p_1, \ldots, q_n, p_n)$. Then equation (2.49) states that in the Schrödinger representation, the wave functions are the elements of Schwartz space.

The uniqueness theorem enables us to see that it is not the Schrödinger representation which is important, but any s–class representation will do just as well.

It remains to consider the possibility that if we add other physically relevant operators to the list $q_1, p_1, \ldots, q_d, p_d$, the space of wave functions will be a proper subspace of Schwartz space.

In Chapter 6 we shall prove that if we add in the Hamiltonian, nothing changes—at least for the class of potentials we use. If we add in the angular momentum, nothing will change either, as it is a polynomial function of the position and momenta operators.

We take it as axiomatic that this is the general situation; the coordinates and momenta and the Hamiltonian are the basic observables.

The reader will recognize that these considerations lie at the heart of the model. We use the basic measurement principle and the canonical commutation relations to determine the space of wave functions, choosing the maximal space. In Chapter 4 we shall see that the choice of wave function space determines the algebra of observables, again up to a maximality choice. This in turn determines the states by duality. Finally, the measurement processes allowed by the theory are based on linear transformations preserving the space of states.

Coming back to the existence of a Fock vector, equations (2.2) and (2.45), we can now fill in the remaining step in the argument. In the Schrödinger representation, the generator of Γ, equation (1.4), is now seen to be generated by the number operator, as indicated previously. Hence the Gaussian, equation (2.45), is invariant. A calculation then shows that the Gaussian has precisely the minimum uncertainty properties demanded in equation (1.3). By the uniqueness theorem, this carries over to any irreducible s-class representation. For reducible representations, this holds in each irreducible sector. ■

The position and momentum operators in the Schrödinger representation are generators of unitary groups. These groups were proposed by Weyl as a means of bypassing problems associated with unbounded operators. Analogous groups exist in all equivalent representations.

2.26 Proposition The self adjoint extensions of the position and momentum operators generate the strongly continuous unitary representations of the group $\mathbb{R}^d$ given by

$$[U_{\mathbf{a}}u](\mathbf{x}) = \exp(i\mathbf{a}\cdot\mathbf{x})u(\mathbf{x}) \tag{2.51.a}$$

and

$$[V_{\mathbf{b}}u](\mathbf{x}) = u(\mathbf{x}+\mathbf{b}). \tag{2.51.b}$$

These groups satisfy the integrated form of the *ccr*, which we shall refer to as the Weyl relations:

$$V_{\mathbf{b}}U_{\mathbf{a}} = U_{\mathbf{a}}V_{\mathbf{b}}\exp(i\mathbf{a}\cdot\mathbf{b}). \tag{2.51.c}$$

Let $\mathtt{A}_S$ be the C^*–algebra obtained by completing the *–algebra of all polynomials in these group elements with respect to the operator norm on $L^2\left(\mathbb{R}^d\right)$. Then $\mathtt{A}_S$ is irreducible.

Proof The Weyl relations follow by computation from the *ccr* . To prove the irreducibility, let $A \in \mathtt{A}'_S$ be an element of the commutant. Now commutation with the group $V\left(\mathbb{R}^d\right)$ means that we can write A in the kernel form

$$[Au](\mathbf{x}) = \int_{\mathbb{R}^d} K(\mathbf{x}-\mathbf{y})u(\mathbf{y})\,d\mathbf{y}.$$

As a two variable function, K must be supposed to be a tempered distribution. Commutation with the group $U\left(\mathbb{R}^d\right)$ implies that K is in fact proportional to the delta function distribution. We conclude from this that $A = cI$, and we are done. ■

As the generators of the Weyl groups constitute an s-class representation–the proof is obvious–we may restate the theorem as follows : s-class representations are those which are in one–to–one correspondence with those of the Weyl groups.

There are two things about the Weyl relations which are worth emphasizing. First, if we define

$$W(\mathbf{z}) = U_{\mathbf{a}}V_{\mathbf{b}}\exp\left(-i\mathbf{a}\cdot\mathbf{b}/2\right),$$

where $\mathbf{z} = \mathbf{a} + i\mathbf{b}$, then W is a projective representation of the additive group of $\mathbb{C}^d$:

$$W(\mathbf{z}_1)W(\mathbf{z}_2) = W(\mathbf{z}_1 + \mathbf{z}_2)\exp\left(i\,\mathrm{Im}\,\mathbf{z}_1\cdot\mathbf{z}_2/2\right).$$

The phase factor is a symplectic form, and this relates quantum mechanics to symplectic geometry.

Second, the Weyl group W may be used to generate a C^*–algebra of the *ccr* for d degrees of freedom. To be more precise, let us now very briefly describe an abstract C^*–algebra of the *ccr* independently due to Slawny [1] and Manuceau [1], following on the work of Segal [1]. The construction is easily generalized to infinitely many degrees of freedom. As the bounded operator approach to algebraic quantum mechanics is well represented in texts, eg, Bogolubov et al [1], Bratteli and Robinson [1], Dubin [1], Emch [1], Ruelle [1], we refer to the literature for elaboration and proofs.

2.27 Proposition Following Segal we complexify the Weyl relations by considering the additive group $\mathbb{C}^d$ and the symplectic form on it obtained as the imaginary part of the usual inner product:

$$\sigma(z,w) = (1/2)\,\mathrm{Im}\langle z,w\rangle. \tag{2.52}$$

By $\mathtt{A}^{(0)}$ we mean the linear space of functions from $\mathbb{C}^d \to \mathbb{C}$ of finite support, equipped with the twisted product

$$[F\star G](z) = \sum\nolimits_{w\in\mathbb{C}^d} F(w)G(z-w)\exp\left(i\sigma(w,z)\right) \tag{2.53.a}$$

and involution

$$F^*(z) = \overline{F(-z)}. \qquad (2.53.b)$$

It is necessary to introduce an auxiliary norm,

$$\|F\|_1 = \sum\nolimits_{w \in \mathbb{C}^d} |F(w)| \qquad (2.54)$$

with respect to which $\mathtt{A}^{(0)}$ is a normed *–algebra . Write $\mathtt{A}^{(1)}$ for its completion.

By an admissible representation of this Banach *–algebra we mean a nondegenerate representation π for which the mapping $t \to \pi(e_{tz})$ is continuous from $\mathbb{R}$ to the weak operator topology. Here we use the elements

$$e_z(w) = \delta_{z,w}, \qquad (2.55)$$

which constitute a Hamel basis for $\mathtt{A}^{(0)}$.

The desired C^*-norm can now be defined as the supremum over all admissible representations:

$$\|F\| = \sup \|\pi(F)\|, \qquad (2.56)$$

and $\mathtt{A}$ as the completion of $\mathtt{A}^{(1)}$ with respect to it. The Stone and von Neumann uniqueness theorem (Putnam [1], Taylor [1]) may be restated as asserting that: *every admissible irreducible cyclic representation of* $\mathtt{A}$ *is unitarily equivalent to the Schrödinger – Weyl algebra* $\mathtt{A}_S$*. Reducible representations on separable spaces are countable direct sums of these.*

By cyclic we mean here that there exists a normalized vector Ω in the representation space such that $\pi(\mathtt{A})\,\Omega$ is dense in $\mathcal{H}$. By irreducible we mean that if a bounded operator on the Hilbert space commutes with all the operators of $\pi(\mathtt{A})$, it must be proportional to the identity operator. We have already introduced these terms for s-class representations ; in later chapters we shall redefine them so that they hold for representations of general locally convex algebras.

We note that the connection to our previous work is that for the Schrödinger representation, denoted π_S, we have the formula

$$\pi_S(e_{\mathbf{z}}) = U_{\mathbf{a}} V_{\mathbf{b}} \exp(-i\mathbf{a} \cdot \mathbf{b}/2), \qquad (2.57)$$

where $\mathbf{z} = \mathbf{a} + i\mathbf{b}$. ■

Lest the above uniqueness theorems lead to misunderstanding, we present some examples very different from the Schrödinger representation.

2.28 *CCR* **Examples** (a) In physics text books the model of a particle confined to a bounded interval is studied, under the name of the infinite square well. It is presumed that the forces on the particle are such as to cause this confinement. Of course everyone knows that such absolute confinement is not physically possible. There are cases where very close confinement does occur, and the idealized limit is extremely convenient for calculational purposes. In mathematical terms this idealization takes us out of the s–class, and affords an interesting example.

We take the region of confinement to be $(0, 1)$, so consider the Hilbert space $L^2(0, 1)$ and the domain of smooth functions vanishing near the boundaries. The multiplication operator is now a bounded operator, and the derivative has many self adjoint extensions; choose one. This pair satisfies the *ccr* on the domain but is not equivalent to a sum of s–class representations. Moreover, the corresponding Weyl groups exist but do not satisfy the Weyl form of the *ccr* . Evidently one must be extremely careful in drawing conclusions from idealized models.

(b) One can find operator groups which satisfy the Weyl relation but whose generators do not constitute an s–class representation, by giving up the ray continuity of the groups. Segal [1] gives the following example. The Hilbert space is the set of almost periodic functions on the line whose square moduli have finite invariant mean. The one parameter unitary groups have the same formulæ as for the Schrödinger representation.

(c) An interesting representation of the *ccr* which *is* equivalent to the Schrödinger representation is due to Bargmann, Fock and Segal. The Hilbert space is

$$\mathcal{H} = \left\{ u \in H\left(\mathbb{C}^d\right) : \int_{\mathbb{C}^d} |u(z)|^2 e^{-|z|^2}\, d\mu(z) < \infty \right\}. \tag{2.58}$$

Here $H\left(\mathbb{C}^d\right)$ is the space of entire analytic functions on $\mathbb{C}^d$ and μ is the Lebesgue measure on $\mathbb{C}^d$. The action of the unitary groups is defined to be

$$W(z)u(w) = \exp\left(-|z|^2 + iz \cdot w/2\right)u(w + i\bar{z}/\sqrt{2}). \tag{2.59}$$

The generators are found by differentiation to be

$$q_j = (i/\sqrt{2})(\partial/\partial w_j + w_j) \tag{2.60.a}$$

and

$$p_j = (1/\sqrt{2})(\partial/\partial w_j - w_j). \tag{2.60.b}$$

For a proof that this is an irreducible s–class representation, we refer the reader to Taylor [1].

We might also mention that for infinitely many degrees of freedom, inequivalent representations are typical in applications. For example, states of the ideal Bose gas corresponding to different temperatures and chemical potential lead to inequivalent representations. Moreover, phase transitions are, typically, associated with both inequivalence and sharp change in the covariance of certain symmetry groups (Bratteli and Robinson [1], Dubin [1], Emch [1], Sewell [1], Ruelle [1]. ■

This ends our formal discussion of the representations of the *ccr* for d-degrees of freedom. Before summing matters up in an axiom we have to know how to combine systems of different kinds of particles. This requires a discussion of particle spin, which we introduce by way of the angular momentum. Until further notice we shall assume that we are dealing with N particles of the same type, all moving in $\mathbb{R}^3$, and that this can be described by the Schrödinger representation. We shall have to modify this rule to take the exclusion principle into effect, but it will do for now.

2.8 ANGULAR MOMENTUM AND SPIN

The reader might have noticed that group theory has entered the formalism, albeit by a back door. In considering the integrated form of the position and momentum operators, we constructed the groups U and V which are intertwined unitary representations of the additive group $\mathbb{R}^d$. Equivalently, we have seen that they constitute a projective representation of the additive group $\mathbb{C}^d$.

Although we shall not discuss symmetries until a later chapter, an important representation of the rotation group will be analyzed here. In classical mechanics (Arnold [1]), rotations are generated by the angular momentum, and this carries over to quantum mechanics. With the correspondence principle as a guide, we expect that the quantum angular momentum operator will be formed like the classical expression, but with the quantum position and momentum operators replacing their classical counterparts.

So let us start with one particle, and the Hilbert space $L^2(\mathbb{R}^3)$. Just as in classical mechanics, the rotation group is $SO(3)$, and it acts on $\mathbb{R}^3$ through the usual 3×3 orthogonal matrices. This representation lifts to a representation by unitary operators on $L^2(\mathbb{R}^3)$ in the familiar way.

Consider the three 1-parameter unitary groups corresponding to the subgroups of rotations around the usual Cartesian axes. That is, if $r_j(\theta)$ is the standard matrix for the rotation around the j-axis, then

$$[R_j(\theta)u](\mathbf{x}) = u[r_j(-\theta)\mathbf{x}] \tag{2.61}$$

defines the corresponding unitary group.

By differentiating with respect to θ at $\theta = 0$ we obtain the generators of these groups. Consistency with the classical limit $\hbar \to 0$ is obtained if we define the angular momentum to be $\hbar$ times the generators. In vector cross product notation, then, the quantum angular momentum operators for a particle are defined to be (Thirring [1], Wigner [1])

$$\mathbf{l} = (-i\hbar)\mathbf{r} \times \nabla \tag{2.62.a}$$

$$= \mathbf{r} \times \mathbf{p}. \tag{2.62.b}$$

Hereafter we revert to our usual practice and set $\hbar = 1$. The Cartesian components are conveniently written as

$$l_j = -i\varepsilon_{jkm} x_k \partial / \partial x_m. \tag{2.62.c}$$

By ε_{jkm} we mean the totally antisymmetric Levi-Civita symbol, with $\varepsilon_{123} = 1$. We also employ the summation convention of Einstein, where a repeated index is summed over its range.

These operators are essentially self adjoint on $\mathcal{S}\left(\mathbb{R}^3\right)$, and satisfy a number of interesting commutation relations. Foremost are the rules

$$[l_j, l_k] = i\varepsilon_{jkm} l_m, \tag{2.63}$$

showing that the angular momentum operators constitute a representation of the Lie algebra $so(3)$ on $L^2\left(\mathbb{R}^3\right)$.

If we let $\mathbf{a}$ stand for any of $\mathbf{q}$, $\mathbf{p}$, or $\mathbf{l}$, then we have the compact notation

$$[l_j, a_k] = i\varepsilon_{jkm} a_m. \tag{2.64.a}$$

As well,

$$[l_j, \mathbf{a} \cdot \mathbf{a}] = 0. \tag{2.64.b}$$

The generalization to N particles is straightforward. The Hilbert space is now $L^2\left(\mathbb{R}^{3N}\right)$ and to the k-th particle we associate the angular momentum

$$\mathbf{l}^k = \mathbf{r}^k \times \mathbf{p}^k. \tag{2.65.a}$$

The *total* angular momentum for the system is then the sum of the angular momenta of the individual particles:

$$\mathbf{L} = \sum\nolimits_{k \leq N} \mathbf{l}^k. \tag{2.65.b}$$

The total angular momentum operator is not best considered in terms of general rotations on $\mathbb{R}^{3N}$, as this does not connect readily with the individual particles. Rather, let us write π for the representation of $SO(3)$ on $L^2(\mathbb{R}^3)$ corresponding to one particle rotations, as constructed above. Then for N particles we must consider space rotations as being given by the N-fold tensor product representation

$$\pi^N = \pi \otimes \cdots \otimes \pi$$

on $L^2(\mathbb{R}^{3N})$. The total angular momentum operators are the generators of the Cartesian subgroups of $\pi^N(SO(3))$; and $\mathcal{S}(\mathbb{R}^{3N})$ is a domain of essential self adjointness for them.

Turning now to the spectra of the angular momentum operators, let us begin by considering the one particle case. It is convenient to introduce spherical polar coordinates on $\mathbb{R}^3$, using the longitude and co- latitude as angular coordinates on the unit sphere S^2. The one particle representation π decomposes into irreducible representations π_j, labelled by the integer $j \in \mathbb{N}$.

Our next task is to decompose Schwartz space $\mathcal{S}(\mathbb{R}^3)$ with respect to the spherical polar coordinates. To do this, let V^j be the $2j+1$-dimensional linear space spanned by the spherical harmonics Y^j_m, with m ranging in integer steps from $-j$ to $+j$. Also let $\mathcal{S}^+$ be the Schwartz space in the radial coordinate.

Then

$$\mathcal{S}(\mathbb{R}^3) = \sum\nolimits_{j\geq 0} \mathcal{S}^j, \tag{2.66.a}$$

where we have written

$$\mathcal{S}^j = \mathcal{S}^+ \bigotimes V^j. \tag{2.66.b}$$

We mean the algebraic tensor product here as V^j is finite dimensional. Equation (2.66) is a convenient decomposition of the domain of the Schrödinger representation, as $\mathcal{S}^j$ is stable under the representation π_j.

Consider the elements of $\mathcal{S}^j$ of the form

$$u^j_m(r,\theta,\phi) = Y^j_m(\theta,\phi)u(r) \tag{2.67.a}$$

These vectors satisfy the differential equations

$$l_3 u^j_m = m\, u^j_m, \tag{2.67.b}$$
$$\mathbf{l}\cdot\mathbf{l} u^j_m = j(j+1)u^j_m, \tag{2.67.c}$$

and

$$(l_1 \pm i l_2) u_m^j = \sqrt{j(j+1) \mp m(m+1)}\, u_{m\pm 1}^j . \qquad (2.67.d)$$

We observe that these functions are eigenfunctions both of l_3 and $\mathbf{l} \cdot \mathbf{l}$.

By a relabelling we could consider simultaneous eigenfunctions of $\mathbf{l}\cdot\mathbf{l}$ and any other component of $\mathbf{l}$ in place of l_3. We shall not prove it, but these considerations exhaust the spectra of the angular momenta. That is, the spectra of l_j are $\mathbb{Z}$, and the spectrum of $\mathbf{l} \cdot \mathbf{l}$ is $\{0, 2, 6, 12, \ldots\}$.

It should be noted that $j \in \mathbb{N}$ follows from the requirement that the Y_j^m must be periodic with period 2π in the colatitude. It turns out that this exhausts the irreducible representations of $SO(3)$. But equation (2.63) holds also for the Lie algebra of the universal covering group $SU(2)$ of $SO(3)$. For this general case, irreducible representations exist for all $j \in \mathbb{N}/2$. This fact is important for the description of particle spin below.

We shall not enter into a discussion of the spectra of the angular momenta of N-particle systems. The procedures to do so are clear, namely tensor products of the above representation and reduction into irreducible components. For the purposes of physics this is not enough, however. Certain particular bases in the product representation spaces are important, depending upon what is being measured. A rather elaborate calculus to deal with this has been developed, starting with the pioneering work of Racah and Wigner. An account may be found in the text of Wigner [1].

Particles with angular momentum $\mathbf{L}$ interact with magnetic fields $\mathbf{H}$, the interaction energy being linear, proportional to $\mathbf{L} \cdot \mathbf{H}$. Because of this, the behaviour of beams of charged particles passing through regions of magnetic fields is an important diagnostic technique in quantum theory. In experiments done at the very outset of quantum mechanics, it was discovered in this way that certain particles, notably electrons, protons and neutrons, behaved as though they had an intrinsic angular momentum with $j = \hbar/2$. This internal degree of freedom is known as the *spin*; we say that the above particles have spin 1/2. Pions, in contrast, have spin 0, photons have spin 1, certain exotic elementary particles have spin 3/2, and the quanta of gravitation, if they exist, probably have spin 2.

It will be observed that there are two distinct classes of particles, as their spins are $1/2, 3/2, \ldots$, or their spins are $0, 1, \ldots$. The particles in the first class are known as *Fermions*, those in the second as *Bosons*. The class distinction arises from the fact that Bosons can be described by representations of $SO(3)$, whereas Fermions require representations of the covering group $SU(2)$. The deepest understanding of spin requires a fully relativistic treatment, but there is a nonrelativistic description of spin, due to Pauli, which is adequate for our purposes here.

We note that it is mathematically consistent with the axioms of relativistic quantum field theory to have a third class of particles, the para-particles. These are associated with fields satisfying third order commutation relations. A careful study of experimental elementary particle data indicates that, to date, no such particle has been found to exist (Bogolubov et al [1]).

Pauli's theory [1] for spin 1/2 particles uses the $d\pi_{1/2}$ representation of the Lie algebra $su(2)$. Recall that this representation acts on the space $\mathbb{C}^2$, the well known 2×2 Pauli matrices σ_j constituting a basis for the Lie algebra, $j = 1, 2, 3$.

When spin is taken into account, the Hilbert space for one spin 1/2-particle is now modified from $L^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3) \bigotimes \mathbb{C}^2$. What we previously referred to as an observable A is now to be represented by the operator $A \otimes \mathbf{1}_2$. By $\mathbf{1}_2$ we mean the 2×2 unit matrix.

If we consider rotations in the spin space $\mathbb{C}^2$, then we see that the matrices

$$s_j = \frac{\hbar}{2} \sigma_j \tag{2.68}$$

are the direct analogues of the l_j; for this reason we refer to them as the spin angular momentum operators, or simply the spin operators. Again we revert to $\hbar = 1$.

This identification does not take the spatial aspect of the particle into account, but this is easily done. If the identity operator on $L^2(\mathbb{R}^3)$ is written as I, the spin operators are of the form $I \otimes \sigma_j$. General observables are operators on $L^2(\mathbb{R}^3) \bigotimes \mathbb{C}^2$ and are convergent infinite linear combinations of product operators of the form $A \otimes m$, with A an operator on $L^2(\mathbb{R}^3)$ and m a matrix on $\mathbb{C}^2$.

To supply a distinction we shall refer to $\mathbf{l}$ as the *orbital* angular momentum, although the particle may not be in a state anything like an orbit.

Much of the spin formalism follows that for the orbital angular momentum outlined above. For example, suppose we consider the spin alone; the spatial components can be tensored in subsequently. Corresponding to the spherical harmonics we have the vectors

$$e_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad e_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.69}$$

There are certain physical situations where it is appropriate to interpret e_+ as describing a spin aligned in a definite direction in space (spin up), and e_- as aligned in the opposite direction (spin down). This direction may, for example, be determined by an external magnetic field. As spin is an essentially quantum mechanical observable, there will also be states without any definite spin orientation.

The spin vectors satisfy the equations

$$s_3\, e_\pm = (\pm 1/2)\, e_\pm, \tag{2.70.a}$$

$$\mathbf{s}\cdot\mathbf{s}\, e_\pm = (3/4)\, e_\pm. \tag{2.70.b}$$

Let us define what are known as the spin raising and lowering operators,

$$s_\pm = s_1 \pm i s_2. \tag{2.70.c}$$

The appropriateness of the name stems from the equations

$$s_\pm\, e_\mp = e_\pm \tag{2.70.d}$$

$$s_\pm\, e_\pm = 0. \tag{2.70.e}$$

Evidently the spectrum of each s_j is the two point set $\{-1/2, +1/2\}$. That of $\mathbf{s}\cdot\mathbf{s}$ is the singleton set $\{3/4\}$.

We also note the $su(2)$ commutation relations

$$s_j s_k - s_k s_j = (i/2)\epsilon_{jkm}\, s_m. \tag{2.71}$$

We mention without further detail that the Pauli theory extends to spin s particles in an obvious way. The system Hilbert space is now modified to $L^2\left(\mathbb{R}^3\right) \bigotimes \mathbb{C}^{2s+1}$. The spin-$s$ angular momentum operators are the matrix generators of the one parameter rotations around the Cartesian axes in spin space $\mathbb{C}^{2s+1}$.

2.9 COMPOUND SYSTEMS: THE EXCLUSION PRINCIPLE

Up to this point we have not considered how to compound quantum systems in any detail. This is because the presence of spin must be taken into account. The most natural assumption is to start from the tensor product of the subsystem Hilbert spaces, but this is not quite correct. The correction is contained in the principle of the indistinguishability of particles in quantum theory.

The origin of this principle is the uncertainty principle, which we will discuss subsequently. For now let us accept that the accuracy of a simultaneous measurement of the position and momentum of a particle is constrained by the Heisenberg inequality, cf, equation (1.2):

$$\Delta_T(q_j)\Delta_T(p_k) \geq (\hbar/2)\, \delta_{jk}. \tag{2.72}$$

This is a direct result of the *ccr* and the interpretation of the theory mentioned in the previous chapter. This is very well known and derived in detail in most physics texts on quantum theory. Granting all this, a very important consequence is immediate :

in quantum theory particles do not have dynamical paths.

For a path has the characteristic property that every point on it is exactly known, and the velocity at every such point is exactly known. But this is precisely what the uncertainty principle forbids.

Another important physical consequence of the theory concerns the individuality of particles. Consider a system of two particles of the same sort, such as electrons. Suppose that at some instant an exact measurement of the position of each is made. This is certainly possible if we do not attempt to measure their momenta simultaneously.

One now attempts to label them on the basis of the result: say particle 1 is at point $\mathbf{x}_1$ and 2 is at $\mathbf{x}_2$. A short time later another measurement of the positions is made, and it is observed that there is a particle at $\mathbf{x}_3$ and another at $\mathbf{x}_4$. In order to know whether it is particle 1 or particle 2 at $\mathbf{x}_3$ one would have to know the directions taken by these particles from their previously measured positions. But this is forbidden by the uncertainty principle.

This situation is not avoided by taking the second pair of measurements sooner; there will always be some small duration between measurements, and this is enough. Nor would measuring the position of one particle and the momentum of the other avoid the problem. We conclude that because of the uncertainty principle:

one cannot distinguish between identical particles.

If we grant that pure states are associated with wave functions through

$$T(a) = \langle u, au \rangle,$$

notice that the phase factor substitution $u \to e^{i\theta}u$ does not change the expected value. From the irreducibility property, moreover, this is the most general class of transformation that will change none of the expected values.

Suppose u represents a state of 2 particles. From the indistinguishability principle, the interchange of the coordinates of the two particles, including spin, must leave all the expected values invariant. This leads us to the symbolic rule

$$u(1,2) = \exp(i\theta_{12})u(2,1). \tag{2.73.a}$$

There is nothing to prevent us from repeating the transposition. Do so, and note that θ_{12} must equal θ_{21}: otherwise we could use the phase factor to distinguish the particles. It follows that

$$u(1,2) = \pm u(2,1). \tag{2.73.b}$$

For N particles, things are not so simple. This is where parastatistics can arise. But if we do not consider such solutions, on the grounds that they do not occur in nature, we are left with totally symmetric or totally antisymmetric solutions. From the axioms of relativistic quantum field theory, it follows that we are not free to choose the sign at will, however. The sign is a consequence of the spin.

By an ingenious analysis of atomic structure data, Pauli [2] discerned that multi-electron wave functions were always antisymmetric. This has the further consequence that no two electrons in the system could be in identical states: this is the famous Pauli exclusion principle. Subsequent analysis showed that this holds for all Fermion systems. Cf also Stoner [1].

Considerations of Boson systems, the ideal Bose gas being a case in point, shows that the opposite parity prevails. This can even favour the occurrence of many Bosons in the same state. In the ideal Bose gas this occurs under the name of condensation, and is responsible for a phase transition at a certain critical temperature.

Another unexpected consequence of these considerations is the mysterious exchange interaction for Fermions. For a pair of atomic electrons, suppose the spin variables have a definite symmetry under particle interchange. It is then necessary that symmetry under interchange of the space variables must "follow suit" so as to achieve total antisymmetry.

If the energy operator for these electrons does not contain the spin explicitly, as is usually the case in atomic physics, the required spatial symmetry causes the allowed energy levels to be modified from that which would be expected on the grounds of spectral analysis alone. It turns out as though an extra, somewhat mysterious, exchange interaction can replace the absent spin so as to achieve the correct result. This effect is by no means small, and is of significant importance in the theory of chemical bonding due to Heitler and London. With a little poetic licence we might say that there could be no organic compounds, hence no life, without these entirely quantum symmetry effects.

Summarizing,

2.29 The Indistinguishability Principle It follows from the *ccr* that quantum particles do not have paths, and so particles of the same species cannot be distinguished.

It is a principle of nature that the wave functions for N particles of a given species are either totally symmetric or totally antisymmetric under the interchange of particle coordinates, including spin, as the particles are either Bosons or Fermions, respectively. This connection between spin and statistics is proved from the Wightman axioms of quantum field theory (Bogolubov et al [1], Streater and Wightman [1]). ■

2.10 TENSOR PRODUCTS AND SYMMETRY

A few remarks concerning the relation between tensor products and the above symmetries are in order here.

Now much of what follows is just multilinear algebra (Greub [1]) with continuity tagged on. Things seem clearer if we adopt a single notation which covers all the cases. It will be axiomatic that we choose the space of wave functions to be a maximal space. Consider a system of N particles moving in space, $\mathbb{R}^3$. Such a system has $d = 3N$ degrees of freedom, and we write $\mathcal{V}_{(N)}$ to mean any of the maximal spaces of an s–class representation of the ccr or its Hilbert space completion.

Next we allow for particle spin. As a first step, let us suppose that all N particles are of the same type, electrons for instance. Then they all possess the same spin s, determined by their type t. We write $\mathcal{V}_{(N,t)}$ for the space $\mathcal{V}_{(N)}$ when spin is included. From our work in §2.8, we deduce that

$$\mathcal{V}_{(N,t)} = \mathcal{V}_{(N)} \bigotimes \left[\bigotimes^{d} \mathbb{C}^{2s+1} \right]. \tag{2.74}$$

Note that as the spin space $\mathbb{C}^{2s+1}$ is finite dimensional, the algebraic tensor product suffices here. For the same reason, tensor products involving $\mathcal{V}_{(N,t)}$ are topologically identical to those involving $\mathcal{V}_{(N)}$ in all cases.

Let us introduce the notation $\mathcal{V}_{(N,\diamond)}$ to stand for either $\mathcal{V}_{(N)}$ or $\mathcal{V}_{(N,t)}$ indifferently, but with the convention that the same choice must be made everywhere in an equation.

We assume that the reader knows what a topological tensor product is, in particular for Hilbert spaces and the projective tensor product topology for locally convex spaces. This subject is described in detail in nearly all the texts on topological vector spaces that we have cited.

2.30 Lemma Let $\widehat{\otimes}$ indicate the completion of the algebraic tensor product in the projective topology for the nuclear Fréchet case and $\otimes_H$ the Hilbert topology in the Hilbert space case. Then the composition law for the spaces $\mathcal{V}_{(N,\diamond)}$ is

$$\mathcal{V}_{(N,\diamond)} \widehat{\bigotimes} \mathcal{V}_{(M,\diamond)} \cong \mathcal{V}_{(N+M,\diamond)}. \tag{2.75.a}$$

Now each single particle is associated with three degrees of freedom, $d = 3$, and as we are considering N particles, the following special case of equation (2.75.a) is important:

$$\mathcal{V}_{(N,\diamond)} = \widehat{\bigotimes}^{N} \mathcal{V}_{(1,\diamond)}. \tag{2.75.b}$$

Proof This is a completely standard result for $\mathcal{S}(\mathbb{R}^n)$ and $L^2(\mathbb{R}^n)$, Trèves [1]. The inclusion of the finite dimensional spin spaces will not change matters, as noted above. ■

Equation (2.75.b) indicates how the *ccr* representation space for N particles would be obtained from that of N 1–particle spaces were there no indistinguishability principle. In order to satisfy this principle we must extract the symmetric and antisymmetric subspaces of $\mathcal{V}_{(N,,\diamond)}$, which is accomplished by the following standard technique of multilinear algebra.

Let the permutation group on N letters, G_N, act on $\mathcal{V}_{(N,\diamond)}$ by the rule

$$T_g u(1, 2, \ldots, N) = u(g^{-1}1, g^{-1}2, \ldots, g^{-1}N), \qquad g \in G_N. \tag{2.76}$$

In this notation, the symbol j refers to all the coordinates of particle j, whatever their nature. In the Schrödinger representation, for instance, the coordinates are space and spin.

2.31 Proposition Let $(-1)^g$ stand for the parity of the indicated permutation; it is convenient to define $(+1)^g$ to be unity for all g. Then the symmetrizing and antisymmetrizing operators are defined to be

$$\Lambda_\pm = (N!)^{-1} \sum\nolimits_{g \in G_N} (\pm 1)^g T_g, \tag{2.77}$$

respectively.

If $\mathcal{V}_{(N,\diamond)}$ is a maximal carrier space, each T_g is a continuous open linear operator, and if it is a Hilbert space they are unitary. Then $\Lambda_\pm$ is a continuous idempotent which is symmetric with respect to the inner product, and commutes with the T_g.

The symmetric and antisymmetric N-particle subspaces, defined as their respective ranges, are nuclear Fréchet spaces; we write

$$\mathcal{W}_{(N,\diamond)} = \Lambda_\pm \mathcal{V}_{(N,\diamond)} \tag{2.78.a}$$

$$= \Lambda_\pm \left[\widehat{\bigotimes}^{N} \mathcal{V}_{(1,\diamond)} \right]. \tag{2.78.b}$$

To resolve a possible ambiguity, we note here that we shall take it to be a principle of nature that the + sign will always appear for those types t corresponding to integer spin s, and the − sign for half–integral spin. Mathematically, though, there is no obstruction to taking even and odd projections of any of the carrier spaces.

Proof As the group G_N is finite, it suffices to prove the continuity of each T_g in order to prove $\Lambda_\pm$ continuous. Recall that a basis of seminorms for the projective tensor product topology on $E\bigotimes_\pi F$ is given by the infimum

$$p\otimes_\pi q(\xi) = \inf \sum p(u_j)q(v_j) \tag{2.79}$$

over all such representations of $\xi \in E\bigotimes_\pi F$ of the form $\xi = \sum u_j \otimes v_j$; similarly for any n-factor product. Then

$$[p_1 \otimes_\pi \cdots \otimes_\pi p_n] \circ T_{g^{-1}} = [p_{g(1)} \otimes_\pi \cdots \otimes_\pi p_{g(n)}] \, ,$$

proving the continuity. As

$$(T_g)^{-1} = T_{g^{-1}},$$

T_g is open.

A finite sum of open maps is open, so $\Lambda_\pm$ is open. As $\Lambda_\pm$ are idempotents, their ranges are closed in $\mathcal{V}_{(N,\diamond)}$, and so must be Fréchet . As subspaces of a nuclear space they are nuclear. The other properties are well known from algebra and we omit the proof.

Finally, the proof in the Hilbert space case goes the same way, but using only one value $\mathbf{r} = 0$. ■

Next we extend this formalism to the operators on $\mathcal{W}_{(N,\diamond)}$.

2.32 Proposition (a) Recall that $\mathcal{L}_b(E)$ is the space of continuous linear maps from E to itself, equipped with the strong topology. Then there exists an isomorphism

$$\iota : \widehat{\bigotimes}^N \mathcal{L}_b\left(\mathcal{V}_{(1,\diamond)}\right) \to \mathcal{L}_b\left(\mathcal{V}_{(N,\diamond)}\right) \tag{2.80.a}$$

such that if $A = A_1 \bigotimes \cdots \bigotimes A_N$ is an element of $\widehat{\bigotimes}^N \mathcal{L}_b\left(\mathcal{V}_{(1,\diamond)}\right)$, then

$$\iota(A)(u_1 \otimes \cdots \otimes u_N) = A_1 u_1 \otimes \cdots \otimes A_N u_N \tag{2.80.b}$$

for $u_1, \ldots, u_N \in \mathcal{V}_{(1,\diamond)}$. By a common convention, this isomorphism is usually suppressed, and the symbol ι dropped.

(b) For every $A \in \mathcal{L}_b\left(\mathcal{V}_{(N,\diamond)}\right)$ define

$$\tilde{\Lambda}(A) = A \circ \Lambda_+. \tag{2.81.a}$$

Then $\tilde{\Lambda}(A)$ is a continuous linear map from $\mathcal{L}_b\left(\mathcal{V}_{(N,\diamond)}\right)$ to itself, and satisfies the following identities:

$$\tilde{\Lambda}(A) \circ \Lambda_\pm = \Lambda_\pm A \Lambda_\pm. \tag{2.81.b}$$

Then $\mathcal{W}_{(N,\diamond)} = \Lambda_\pm \mathcal{V}_{(N,\diamond)}$ is invariant under $\tilde{\Lambda}(A)$ for all $A \in \mathcal{L}_b\left(\mathcal{V}_{(N,\diamond)}\right)$. Thus equation (2.81.a) defines a continuous linear map of $\mathcal{L}_b\left(\mathcal{V}_{(N,\diamond)}\right)$ to $\mathcal{L}_b\left(\mathcal{W}_{(N,\diamond)}\right)$.

Applied to the simple operator A, its symmetrized part is

$$\tilde{\Lambda}(A) = (N!)^{-1} \sum_{g \in G_N} A_{g(1)} \bigotimes \cdots \bigotimes A_{g(N)}. \tag{2.81.c}$$

Note carefully that it is the +–symmetrized formula which leaves both ±–symmetrized spaces invariant.

(c) For the unitary one parameter groups generated by the 1-particle position, momentum, angular momentum, raising and lowering operators, and number operators, we take the corresponding N-particle operators to be the symmetric part of the tensor product. This constitutes a continuous representation of these groups on $\mathcal{W}_{(N,\diamond)}$.

Suppose then that $U(t) = \exp(ita)$ is a continuous one parameter group on $\mathcal{W}_{(1,\diamond)}$. The corresponding group on $\mathcal{W}_{(N,\diamond)}$ is the symmetrized tensor product

$$U^{(N)}(t)_+ = \tilde{\Lambda}\left[U(t) \bigotimes \cdots \bigotimes U(t)\right]. \tag{2.82.a}$$

To find the generator, we differentiate formally, and set $t = 0$. Doing this, we find that it to have the somewhat awkward form

$$\begin{aligned} a_+^{(N)} &= a \otimes I \otimes \cdots \otimes I + I \otimes a \otimes I \otimes \cdots \otimes I \\ &\quad + \cdots + I \otimes \cdots \otimes I \otimes a. \end{aligned} \tag{2.82.b}$$

Proof (a) This follows from a standard result in topological vector space theory (Trèves [1]) since the spaces involved are all nuclear Fréchet. Part (b) is true because composition preserves continuity. In part (c), (2.82.a) extends from the space of wave functions to its Hilbert space completion. The extension is strongly continuous, hence differentiable. The derivative is (2.82.b), which evidently restricts continuously to the space of wave functions. ∎

Note that we cannot ascribe the quality represented by a to any particular particle, a consequence of the indistinguishability principle.

These formulas may evidently be generalized to those unitary one-particle groups satisfying the $SNAG$ theorem. With a little more indexing, they may be generalized to groups and operators which are intrinsically multiparticle, for there are such operators; the Coulomb potential between two particles is an example.

We are now in a position to state our next axiom. Our use of the term wave function is not standard, but it has the dual merit of being precise and being consistent with our contention that arbitrary vectors in the Hilbert space of the system cannot occur unless they are in the domain of all the quantum observables. Eventually, we will be able to prove that each normalized wave function determines a pure state of the system.

> **Axiom 2.** Consider an elementary system $\Sigma_{(N,t)}$ consisting of N identical particles of type t, such as electrons, moving in $\mathbb{R}^3$; on physical grounds, the type determines the spin s. By a space of wave functions for the system we shall mean any of the maximal spaces $\mathcal{W}_{(N,t)}[\nu]$ isomorphic to the Schrödinger representation space $\mathcal{S}\left(\mathbb{R}^{3N}\right)_s^{\pm}$, in an obvious notation. The $\pm$ sign is chosen to be $+$ for Bosons and $-$ for Fermions, that is, as $2s+1$ is odd or even. The Hilbert space for the system will then be isomorphic to $L^2\left(\mathbb{R}^{3N}\right)_s^{(\pm)}$. Consider a compound system consisting of N_1 identical particles of type t_1 with spin $s_1,\ldots,$ N_n identical particles of type t_n with spin s_n. Let us write N for the n-tuple $(N_1,\ldots,N_n)$, and similarly **t**, **s** for the type and spin, respectively. Such a system is indicated by the notation
>
> $$\Sigma_{(\mathbf{N},\mathbf{t})} = \Sigma_{(N_1,t_1)} \bigotimes \cdots \bigotimes \Sigma_{(N_n,t_n)}. \tag{2.83}$$
>
> The space of wave functions for the compound system is the completed projective tensor product of the subsystem wave function spaces; there are no symmetry constraints between particles of different types. We write
>
> $$\mathcal{W}_{(\mathbf{N},\mathbf{t})} = \widehat{\bigotimes}_{j=1}^{n} \mathcal{W}_{(N_j,t_j)}; \tag{2.84}$$
>
> if no misunderstanding is likely, we shall simply write $\mathcal{W}$. This compound system has
>
> $$3N_1(2s_1+1)+\cdots+3N_n(2s_n+1)$$
>
> degrees of freedom. In all cases the operators compound according to the rules above, and the wave function spaces are nuclear Fréchet spaces. The choice of $\mathcal{W}$

depends firstly on the identification of the coordinate and momentum operators as the generators of the Weyl unitary groups, generalizing the phase space translations of classical mechanics. Secondly, we take it that these same coordinate and momenta operators constitute the basic observables. Combining this with the basic measurement principle that every observable is measurable in every state, we arrive at

$$\mathcal{S}\left(\mathbb{R}^d\right) = \mathcal{C}^\infty\left(q_1, p_1, \ldots, q_d, p_d\right),$$

before including spin and statistics. These are included through the Pauli scheme. ∎

In what follows it will prove convenient to refer to a maximal space carrying an s–class representation of the *ccr* and equipped with its nuclear Fréchet ν- topology simply as a maximal space.

We end this section with a structure theorem for the space of wave functions. For one particle without spin, equation (2.28) gives a representation in terms of a number operator. It turns out that we can do the same thing for the more general systems described in Axiom 2.

2.33 Theorem The space of wave functions for the system $\Sigma_{(N,t)}$ of N identical particles of type t is representable as

$$\mathcal{W}_{(N,t)}[\nu] = \mathcal{C}^\infty\left(\mathrm{M}_{(N,t)}\right). \tag{2.85}$$

From now on we shall write

$$\mathrm{M}_{(1)} = M_1 + M_2 + M_3, \tag{2.86.a}$$

on the relevant domain in $L^2\left(\mathbb{R}^3\right)$, for the indicated self adjoint number operator associated with one particle when spin has not been taken into account; and

$$\mathrm{M}_{(1,t)} = \mathrm{M}_{(1)} \otimes I_s \tag{2.86.b}$$

on $L^2\left(\mathbb{R}^3\right) \bigotimes \mathbb{C}^{2s+1}$ when it has. Here I_s is the identity operator on $\mathbb{C}^{2s+1}$. This covers the case of one particle of type t, with spin s.

For N particles of type t, the number operator obtained from equation (2.81) has the appropriate dense domain in the Hilbert space

$$\bigotimes\nolimits_{\pm}^{N}\left[L^2\left(\mathbb{R}^3\right) \bigotimes \mathbb{C}^{2s+1}\right],$$

the $\pm$ choice determined by s as usual; and formula

$$\mathrm{M}_{(N,t)} = \tilde{\Lambda}_{+} \bigotimes^{N} \left[\mathrm{M}_{(1,t)}\right]. \tag{2.86.c}$$

Here, $\tilde{\Lambda}_{+}$ is the $+$ symmetrizing operator, now acting on the indices of the operators, as the $+$ symmetrized form leaves both $\pm$ symmetrized subspaces invariant. In the case at hand, the N-fold tensor product of the same operator is already symmetric, and we have included the symmetrizer symbol for emphasis only.

The corresponding $\nu_{(N,t)}$-topology is determined by the Hilbertian seminorms

$$\begin{aligned} \|x\|_{(N,t);r} &= \left\| \left[\mathrm{M}_{(N,t)}\right]^{r} x \right\|. && (2.87.a) \\ &= \left\langle \left[\mathrm{M}_{(N,t)}\right]^{r} x, \left[\mathrm{M}_{(N,t)}\right]^{r} x \right\rangle^{1/2}, && (2.87.b) \end{aligned}$$

all $x \in \mathcal{W}_{(N,t)}$, and $r \in \mathbb{N}$.

Setting $r = 0$ gives the rigged Hilbert space structure

$$\mathcal{W}_{(N,t)} \subseteq L^{2}_{\pm}\left(\mathbb{R}^{3N}; \mathbb{C}^{2s+1}\right) \subseteq \left[\mathcal{W}_{(N,t)}\right]'. \tag{2.88}$$

For the compound system $\Sigma_{(\mathbf{N},\mathbf{t})}$ described in the Axiom, involving different types of particles, an analogous representation holds. For each type t_j, with $1 \leq j \leq n$, the representation of equation (2.86) is chosen. In compounding the different types, the completed projective tensor product of these representations is taken, with no symmetry requirements. This leads to the result

$$\mathcal{W}_{(\mathbf{N},\mathbf{t})} = \mathcal{C}^{\infty}\left(\bigotimes_{j=1}^{n} \mathrm{M}_{(N_j,t_j)}\right). \tag{2.89}$$

We note that the various number operators all have discrete spectra, with eigenvectors obtained as tensor products of the single particle Hermite eigenvectors, $\pm$ symmetrisation as appropriate. ■

We omit the proof in spite of the apparent complexity of the result as it is evidently a copy of things we have done above, but with more variables to keep account of. There is one new idea which is useful in the proof, however, which is that for nuclear Fréchet spaces the projective tensor product topology is obtainable by using the seminorms of the Hilbertian tensor product topology. Explicitly, if E and F are nuclear Fréchet spaces and

$$p = \langle \cdot, \cdot \rangle_{E}^{1/2}, \qquad q = \langle \cdot, \cdot \rangle_{F}^{1/2}$$

are continuous Hilbertian seminorms, the seminorms of the Hilbertian topology are of the form

$$[p \otimes_h q](u) = \left[\sum_{j,k=1}^{n} \langle x_j, x_k \rangle_E \langle y_j, y_k \rangle_F \right]^{1/2}, \tag{2.90.a}$$

where

$$u = \sum_{j=1}^{n} x_j \otimes y_j. \tag{2.90.b}$$

These seminorms are often very useful for computations, as is the case here. The reason this is so is that this Hilbertian tensor product topology is finer than the injective, and coarser than the projective tensor product topologies. For nuclear Fréchet spaces, however, these latter topologies are equivalent (Trèves [1]).

2.11 QUANTUM CANONICAL TRANSFORMATIONS

As all these maximal spaces are isomorphic, the question arises as to why we distinguish between them at all. The short answer is that mathematical and physical equivalence are not identical. In some cases, different maximal spaces correspond to different diagonal operators. These representations are appropriate to different physical situations. A number of interesting examples are found in Heisenberg [2].

The most important example is $\mathcal{S}\left(\mathbb{R}^{3N}\right)$, on which the position operators are multiplication operators. This is the Schrödinger representation.that we studied above. Applying the Fourier transform, we get a representation in which the momentum operators are diagonal. This is known to physicists as the momentum representation.

The number operator is diagonal on $s^{(3N)}$. By Fourier series we can transform this to a representation in which a *phase* operator is diagonal. Another example, perhaps less physical, is the Bargmann representation, Example 2.28.*c*. Here the raising operator is diagonal. These examples lead us to conclude that the different maximal spaces are to be considered as realizing the quantum mechanical formulation of canonical transformations. Let us elaborate this idea.

The reader will recall that the modern, coordinate free formulation of classical mechanics starts with a smooth manifold, the generalized position space. More important for mechanics is its cotangent manifold, which is the phase space of the system.

The dynamics appear as the flows associated with the Hamiltonian, which is a smooth function on phase space. The acceptable coordinate transformations on phase space are those under which the dynamical flow is invariant, obviously. These are the canonical transformations.

More precisely, and for one degree of freedom, a transformation of coordinates on phase space

$$(q,p) \to (Q,P) \tag{2.91}$$

is a canonical transformation if it is a diffeomorphism and leaves the canonical 2-form invariant:

$$dq \wedge dp \to dQ \wedge dP. \tag{2.92}$$

Of importance for quantum theory is the result that the Poisson bracket is invariant under canonical transformations, cf, Arnold [1].

Dirac has emphasized that the commutator between a large class of quantum observables is "equal" to the Poisson bracket between their classical analogues, multiplied by ih. (See the remarks in the Physical Scholium above.) It follows that the quantum analogue of the classical canonical transformation will be transformations of the quantum algebra which preserve the *ccr* . In our formulation, the precise form of this notion can be given.

2.34 Definition By a quantum canonical transformation we mean a *tvs* isomorphism $T : E_M \to F_M$ between maximal spaces which preserves the s–class structure as specified in Proposition 2.19. ■

As we know, such a transformation T extends to a unitary transformation between the Hilbert space completions of the maximal spaces.

Too many physics texts assert that *all* unitary transformations between Hilbert spaces are canonical, but this cannot be true in such general form. That this is so has always been clear to careful authors, eg, Kemble [1]. To preserve the s–class nature of the *ccr* requires the stability of the domain and the preservation of the continuity of the raising and lowering operators in the ν-topology as well as a formal preservation of the commutation equation. Fourier transformations afford an example of this. In contrast, here is a simple class of counter-examples.

2.35 A noncanonical transformation Consider one degree of freedom, let f be a continuous real function on $\mathbb{R}$, and set

$$[Uh](x) = \exp(if(x))h(x), \tag{2.93}$$

for all $h \in \mathcal{S}(\mathbb{R})$. If f is continuous but not smooth, or if it grows too fast at infinity, then U is a unitary operator under which $\mathcal{S}(\mathbb{R})$ is not stable. For example, $f(x) = |x|$ will do.

The commutation equations still formally hold, as

$$q \to q \qquad \text{and} \qquad p \to p - f'. \tag{2.94}$$

Note that in our example, f' is discontinuous. ■

In sum, then, the different maximal spaces are associated with the quantum canonical transformation scheme. Definition 2.34 is the translation of Dirac's transformation theory [2] into our model.

3. TOPOLOGICAL ALGEBRAS

3.1 ALGEBRAS

Our *algebra of observables* will be a noncommutative topological *-algebra, whose topology will not be normable; it will not even be barreled. Such algebras are not widely known, and their theory is relatively poorly developed, in general. As we shall be using a number of aspects of what theory there is, we felt it useful to include a discussion of the subject as a topic in its own right.

In this chapter we do this, occasionally contrasting the non normed and the normed cases. We also have introduced certain classes of non normed algebras as interesting in their own right.

We shall start our discussion at a fairly general level, and quickly proceed to the interesting classes. We impose one important condition from the outset, however : *all algebras will be over the complex field*, unless the real field is mentioned explicitly. This immediately places the discussion on the analysis road, turning off from algebra and ring theory *per se*. We begin with some necessary basic definitions.

3.1 Definition (a) A real (respectively complex) algebra $\mathcal{A}$ is a real (respectively complex) vector space equipped with an associative product which is distributive over addition. With respect to addition and the product, $\mathcal{A}$ is an associative ring.

If $xy = yx$ for all pairs of elements, we say that $\mathcal{A}$ is commutative or, synonomously, abelian.

An identity for the algebra is an element $e \in \mathcal{A}$ satisfying $xe = ex = x$ for all elements $x \in \mathcal{A}$. Such an element is unique if it exists at all, and an algebra with an identity will be said to be unital.

(b) By a *–algebra we mean a complex algebra $\mathcal{A}$ equipped with an involution $x \to x^*$. An involution is an antilinear operator on $\mathcal{A}$ which reverses the product,

$$(xy)^* = y^* x^*, \tag{3.1.a}$$

and satisfies

$$(x^*)^* = x. \tag{3.1.b}$$

In a unital algebra,

$$e^* = e. \tag{3.1.c}$$

The involution on a *–algebra defines the real linear subspace,

$$\mathcal{A}_h = \{ x \in \mathcal{A} : x = x^* \}, \tag{3.2}$$

whose elements are said to be hermitian. We refer to $\mathcal{A}_h$ as the hermitian part of $\mathcal{A}$. The hermitian subspace is an algebra iff $\mathcal{A}$ is abelian.

Given $a \in \mathcal{A}$, define

$$a_1 = (a + a^*)/2 \qquad \text{and} \qquad a_2 = (a - a^*)/2i. \tag{3.3.a}$$

The inverse

$$a = a_1 + ia_2 \qquad \text{and} \qquad a^* = a_1 - ia_2 \tag{3.3.b}$$

provides a unique decomposition

$$\mathcal{A} = \mathcal{A}_h + i\,\mathcal{A}_h. \tag{3.4}$$

(c) By a topological algebra we mean an algebra which is a topological vector space such that the product is *separately* continuous.

(d) A *-algebra which is a topological algebra is said to be a topological *-algebra if the involution is a continuous map. ■

Given a nonunital algebra, it is sometimes convenient to add an identity to it. This is achieved by the following standard construction.

3.2 Adjunction of an Identity Let $\mathcal{A}$ be an algebra, and consider the direct sum

$$\mathcal{A}^{\oplus} = \mathcal{A} \bigoplus \mathbb{C}. \tag{3.5.a}$$

This linear space is a unital algebra when equipped with the product

$$(x, a) \cdot (y, b) = (xy + bx + ay, ab); \tag{3.5.b}$$

the identity is $(0, 1)$.

When $\mathcal{A}$ is a topological algebra, we equip $\mathcal{A}^{\oplus}$ with the direct sum topology, and this turns it into a unital topological algebra.

A disadvantage of this construction is that if $\mathcal{A}$ already has an identity, its image in $\mathcal{A}^{\oplus}$ cannot be identified with $(0, 1)$. ■

It will be our practice to refer to a topological algebra which is a *tvs* of a particular class as topological algebra of that class. Hence one has locally convex algebras, Banach algebras, and so on. Many of the results given below are valid both for topological algebras and topological *-algebras. It is convenient to have a common notation for both cases, and we choose to write $^\diamond$–algebra . Hence, *eg* , a $B^\diamond$–algebra is a topological $^\diamond$–algebra which is a Banach space. Another standard terminology concerns mappings. We use the terms algebraic homomorphism and isomorphism to indicate the preservation of the algebraic structure. When the topological structure is preserved as well, we indicate the topological status of such maps explicitly. Thus, a continuous homomorphism is a homomorphism which is a continuous linear mapping between the topological linear structures. Similarly, a topological isomorphism is an algebra isomorphism which is linearly bicontinuous. Sometimes we wish to specify a map referring only to the linear structure; we do so by including the term *linear* explicitly. Finally, there will be instances where the context will be trusted to indicate exactly what is being preserved.

We assume the reader to be familiar with the basic substructures of an algebra: left, right, and two sided ideals, and subalgebras. For topological algebras we also have closed variants of these, with obvious meanings. A closed subalgebra, then, is a subset of a topological algebra which is both a subalgebra and a closed linear subspace. The closure of a subalgebra (respectively ideal) is a closed subalgebra (respectively closed ideal).

It should be noted that the completion of a topological algebra is not necessarily an algebra, let alone a topological algebra. An example is the algebra of polynomials under pointwise multiplication, regarded as a dense subspace of the Banach space $L^1([0,1])$.

Suppose $\mathcal{B}$ is a subset of $\mathcal{A}$, and is such that

$$x \in \mathcal{B} \qquad \Leftrightarrow \qquad x^* \in \mathcal{B}. \tag{3.6}$$

Then $\mathcal{B}$ is said to be stable under involution, or *-symmetric.

Analogously, a *-homomorphism φ is an algebra homomorphism such that

$$\varphi(x)^* = \varphi(x^*). \tag{3.7}$$

We note that a *-ideal is necessarily two sided.

For algebras, homomorphisms are characterized as follows.

3.3 Proposition The kernel $\mathcal{K}$ of a homomorphism φ of an algebra $\mathcal{A}$ is a two sided ideal, and the image of the algebra $\mathcal{A}$ under the homomorphism φ is isomorphic to the quotient algebra $\mathcal{A}/\mathcal{K}$. Conversely, if $\mathcal{K}$ is any two sided ideal in $\mathcal{A}$, the quotient map $\mathcal{A} \to \mathcal{A}/\mathcal{K}$ is a homomorphism whose kernel is $\mathcal{K}$.

If $\mathcal{A}$ is a *–algebra , the above remains true if φ is a *-homomorphism and $\mathcal{K}$ a *- ideal. If $\mathcal{A}$ is a Hausdorff topological $^\diamond$–algebra , the above algebraic relations remain true if φ is a continuous $^\diamond$- homomorphism and $\mathcal{K}$ a closed $^\diamond$- ideal. Moreover, the algebraic isomorphism $\mathcal{A}/\mathcal{K} \to \operatorname{Im}\varphi$ is continuous. Conversely, the quotient map $\mathcal{A} \to \mathcal{A}/\mathcal{K}$ is continuous and open.

Proof The algebraic material can be found in any algebra text, eg, Greub [1]. The topological properties are properties of the quotient topology, cf, Jarchow [1]. ■

3.4 Function Spaces Let X be any nonvoid set and $\mathbb{C}^X$ the set of all mappings $f : X \to \mathbb{C}$. This is an abelian unital *–algebra when equipped with the pointwise operations

$$[f+g]\,(x) = f(x) + g(x), \tag{3.8.a}$$

$$[\lambda f]\,(x) = \lambda\,[f(x)]\,, \tag{3.8.b}$$

$$[fg]\,(x) = f(x)g(x), \tag{3.8.c}$$

$$[f^*]\,(x) = \overline{f(x)}. \tag{3.8.d}$$

The identity is the constant function $e(x) = 1$ for all $x \in X$.

This algebra is not usually encountered in analysis, as no topological constraints have been placed on the class of functions. An example of a useful subalgebra of $\mathbb{C}^X$ which does appear in analysis is the LF- space $\mathcal{D}\,(\mathbb{R})$ of smooth functions of compact support. Here we have taken $X = \mathbb{R}$, but other choices are possible, *eg* , any nonempty open subset of $\mathbb{R}^d$.

Unless otherwise specified, this space will carry its usual topology, which is the strict inductive limit

$$\mathcal{D}\,(\mathbb{R}) = \lim\,\mathrm{ind}_{n\to\infty}\,\mathcal{C}_c^\infty\,(K_n) \tag{3.9}$$

of smooth functions with support in the compact subsets K_n. These are chosen so that K_n is a subset of the interior of K_{n+1}, and the chain ascends to $\mathbb{R}$.

We note that each $\mathcal{C}_c^\infty\,(K_n)$ is a non–normable Fréchet space, and the strict inductive limit is not metrizable. As the identity function is not of compact support, and taking into account some known linear properties, $\mathcal{D}\,(\mathbb{R})$ is a nonunital nonmetrizable nuclear LF *-algebra, cf, Trèves [1]. ■

We shall meet a number of other examples in the following text.

In accordance with our conventions, a topological $^\diamond$–algebra which is a locally convex space is known as a locally convex $^\diamond$–algebra. This is the most general class that will concern us. We note that this class becomes a category when we take as morphisms the continuous $^\diamond$–algebra homomorphisms.

It is shown, eg, in Naimark [1], §II.8, that in this category, topological closure preserves the basic structures we mentioned in the previous section: left, right and two sided ideals, and or right ideals, and subalgebras, both *-symmetric and not. It is also indicated there that this category is stable under the adjunction of the identity. We omit the simple proof.

No completely general relation between the product and the topology is known, but these next results are quite useful.

3.5 Proposition (a) The product on a barreled topological $^\diamond$–algebra $\mathcal{A}$ is hypocontinuous. That is, for any bounded set $\mathcal{B} \subset \mathcal{A}$ and any continuous seminorm p, there exists a continuous seminorm q such that

$$p(xy) \leq q(y) \qquad \text{and} \qquad p(yx) \leq q(y) \qquad \text{for all } x \in \mathcal{B},\, y \in \mathcal{A}. \tag{3.10}$$

(b) For all Baire metrizable algebras the product is jointly continuous. This class includes all Fréchet algebras.

(c) Let $\mathcal{A}$ be a locally convex algebra whose product is jointly continuous. Then the completion of $\mathcal{A}$ is a locally convex algebra with a jointly continuous product.

(d) Let $\mathcal{A}$ be a topological $^\diamond$–algebra, and U a subset which is a closed barrel, ie, absolutely convex, closed and absorbing. Let p be its gauge seminorm. Then if p is submultiplicative,

$$p(xy) \leq p(x)\,p(y), \tag{3.11.a}$$

U is idempotent, meaning that

$$U \cdot U \subseteq U. \tag{3.11.b}$$

Conversely, if U is an idempotent barrel, its gauge is a seminorm which is submultiplicative.

Proof Every separately continuous bilinear map

$$E \times F \to G,$$

where E and F are barreled and G is locally convex, is hypocontinuous, cf, Trèves [1], Theorem 41.2. This proves (a).

If in addition E and F are Baire metrizable spaces, the map is jointly continuous, cf, Schaeffer [1], III.5.1, showing (b).

(c) This follows from the analogous result for rings, cf, Bourbaki [1], III.6.5.

(d) is elementary, and we omit a proof. ■

The general situation is that the product is separately continuous, and no other properties hold. The property of being barreled is fairly typical in applications, hence so is hypocontinuity of the product. Unfortunately, this is not the case for the algebra of observables, which is described in the next chapter.

There are a number of different subclasses of locally convex algebras which have been studied for their intrinsic mathematical interest. The following example is a case in point. This class is defined by raising the submultiplicative property (3.11.a) to the fore. As this property is characteristic for norms, we may expect such an algebra to be a sort of localized normed algebra.

3.6 Locally Multiplicatively Convex Algebras A topological algebra for which the topology may be defined by a family of submultiplicative seminorms is known as a locally multiplicatively convex algebra, usually abbreviated to lmc-algebra.

From the above proposition we see that we can find a basis of neighbourhoods of the origin in an lmc-algebra consisting of idempotent barrels. We also see that the product is jointly continuous. This class was introduced by Arens [1].

The basic structural theorem was found by Michael [1]. The reader will recall that every complete locally convex space E can be represented as the projective limit of Banach spaces. These Banach spaces are the closures in the quotient norm of $E/p^{-1}(0)$, as p runs over a defining family of seminorms. The point of the theorem is that these Banach spaces can be taken to be algebras. For a general locally convex algebra, this is not the case.

Arens - Michaels' Theorem Every complete lmc-algebra is the projective limit of Banach algebras. ■

Here is an example. Let $\mathcal{C}(X)$ be the unital abelian algebra of continuous complex valued functions from a Hausdorff, σ-complete and locally compact space X. Equip it with the compact open topology, which is defined by the following family of seminorms:

$$p_K(f) = \sup_{x \in K} |f(x)| \tag{3.12}$$

as K runs over the compact subsets of X.

With this topology $\mathcal{C}(X)$ is a complete lmc-algebra. It is a Fréchet lmc-algebra if and only if X possesses a countable total family of compact subsets; this property goes under the name of hemicompactness. Finally, it is a Banach algebra if and only if X is compact. ■

The class of algebras which has received the most investigation is undoubtedly the normed algebras, with its important subclasses of C^*-algebras and W^*- algebras. For the purposes of this book, these classes play the role of an understudy, so to speak, remaining in the wings, but not often appearing. For comparison's sake we include the following material, which stands in contrast with various properties of the non-normed algebras encountered below. Standard references are Bratteli and Robinson [1], Dixmier [1-2], Kadison and Ringrose [1], Pedersen [1], Sakai [1], Takesaki [1].

With our standard convention, a normed $^\diamond$–algebra , respectively a Banach $^\diamond$–algebra , is a topological $^\diamond$–algebra which is a normed space, respectively a Banach space. The latter will usually be abbreviated to $B^\diamond$–algebra .

These definitions are consistent with the practice in the theory of locally convex algebras, but are not the ones usually found in most books on functional analysis. This difference is only apparent, as the following shows.

3.7 Lemma Given any Banach algebra $(\mathcal{A}, \|\cdot\|)$, there exists an equivalent norm $\|\cdot\|'$ for $\mathcal{A}$ which is submultiplicative:

$$\|xy\|' \leq \|x\|' \, \|y\|'. \tag{3.13.a}$$

If the algebra is unital, then the norm can be taken to satisfy the condition

$$\|e\|' = 1. \tag{3.13.b}$$

Given any Banach *–algebra , there is an equivalent norm $\|\cdot\|'$ which satisfies both equations (3.13.a,b) and

$$\|x^*\|' = \|x\|'. \tag{3.13.c}$$

Proof As a Banach space is a Fréchet space, we know that the product is jointly continuous; this means that the norm satisfies

$$\|xy\| \leq k\,\|x\|\,\|y\|.$$

Define the auxiliary norm

$$\|\cdot\|'' = k\,\|\cdot\|.$$

This is submultiplicative, but does not necessarily satisfy the normalization condition equation (3.13.b) . For this reason we define

$$\|x\|' = \sup_{y\neq 0} \|xy\|'' / \|y\|''.$$

This is a norm with the required properties. It is also equivalent to the original norm. To see this, we observe that the original norm is obviously equivalent to $\|\cdot\|''$; and it is straightforward to prove that

$$\|x\|'' / \|e\|'' \leq \|x\|' \leq \|x\|''.$$

For a Banach *–algebra this procedure leads to an equivalent norm satisfying equations (3.13.a,b), call it $\|\cdot\|'''$. It remains to satisfy the involution condition in addition. But this is easy; just define

$$\|x\|' = \max\{\|x\|''', \|x^*\|'''\}.$$

■

3.8 The Group Algebra Amongst the many examples of Banach algebras, one of the most interesting is the group algebra $L^1(G)$ of a locally compact group G. This is defined to be the Banach space of equivalence classes of functions $G \to \mathbb{C}$ which are absolutely integrable with respect to the left Haar measure.

The product is taken to be the convolution

$$[x \star y](g) = \int_G x(h)\, y(h^{-1}g)\, d\mu(h). \tag{3.14.a}$$

We define an involution by

$$[x^*](g) = \Delta(g^{-1})\overline{x(g^{-1})}, \tag{3.14.b}$$

where Δ is the modular function on the group.

The group algebra is then a B^*–algebra , with the usual L^1- norm satisfying equation (3.13.a) .

The algebra is abelian if and only if the group is. The algebra is unital if and only if the group is discrete, but in general it contains a two sided approximate identity, *ie* , a net (u_α) of elements of the group algebra which satisfy

$$\lim u_\alpha \star x = \lim x \star u_\alpha = x \tag{3.15}$$

for all elements x of the algebra. ■

The great utility of this algebra is that its nondegenerate representations are in one to one correspondence with the weakly continuous unitary representations of G. For a further discussion of this topic, the reader is referred to Naimark [1] and Reiter [1].

3.9 Cauchy Convolution Algebras An interesting class of algebras can be constructed from certain sequence spaces. In this example all sequences are complex unless otherwise specified. We adopt the notation ω for the vector space of all sequences, and ϕ for the vector space of all terminating sequences. Then a sequence space is a subset of ω containing ϕ which is a complex vector space with respect to pointwise addition and scalar multiplication. Note that ϕ is the space $\phi^{(1)}$ of Definition (2.5.b). As cited before, the basic reference is Köthe [1].

A sequence space λ is said to be a Cauchy convolution algebra if it is closed under the convolution product introduced by Cauchy:

$$(x \star y)_n = \sum_{k=0}^{n} x_{n-k} y_k . \tag{3.16.a}$$

It is a *–algebra with the involution based on complex conjugation:

$$x^* = (\overline{x_k}) . \tag{3.16.b}$$

The first thing we note is that not all sequence spaces are Cauchy convolution algebras. This is the case, for example, for the spaces l^p with $p > 1$, c and c_0. These last two are the spaces of convergent and zero convergent sequences, respectively.

Sequence spaces have a natural topology, known as the normal topology, and defined as follows. For any sequence space λ, we denote by $\lambda^\times$ its Köthe dual, the space of all sequences u in ω for which the sum

$$p_u(x) = \sum_{n \geq 0} |u_n \, x_n| \tag{3.17}$$

is finite for all $x \in \lambda$. It should be noted that $\lambda^\times$ is itself a sequence space.

The function p_u is then a seminorm. The normal topology is defined to be the locally convex topology determined by the family

$$\{ p_u : u \in \lambda^\times \} . \tag{3.18}$$

We denote it by $t(\lambda^\times)$. Then

$$\lambda[t(\lambda^\times)]' = \lambda^\times \tag{3.19}$$

indicates the topological duality relation.

With these definitions, l^1 is a Cauchy convolution algebra which is a B^*-algebra. In essence, this was shown by Cauchy in connection with his researches on divergent series (Hardy [1]).

The sequence space $s^{(1)}$ is also a Cauchy convolution *–algebra . Moreover, it is both Fréchet and nuclear, since the normal topology $t\left([s^{(1)}]^{\times}\right)$ is the same as the usual topology.

Examples of Cauchy convolution *-algebras which are lmc are the l^p for $0 < p < 1$, and the holomorphic spaces

$$h = \left\{ x \in \omega : \lim_{n\to\infty} e^{nk} x_n = 0, \quad \forall k \in \mathbb{N} \right\} \tag{3.20.a}$$

and

$$h_1 = \left\{ x \in \omega : \left(e^{-n/k} x_n\right) \in l^1, \quad \forall k \in \mathbb{N} \right\}. \tag{3.20.b}$$

The names of these last two algebras derive from the fact that the correspondence

$$x \to \sum\nolimits_{n\geq 0} x_n z^n \tag{3.21}$$

is an isomorphism between h and the space $H(\mathbb{C})$ of all entire analytic functions on $\mathbb{C}$, and between h_1 and the space $H(\Delta)$ of all functions holomorphic on the unit disc Δ.

We note that if h and h_1 are given their respective normal topologies, and $H(\mathbb{C})$ and $H(\Delta)$ their respective compact–open topologies, this isomorphism is topological. Furthermore, if $H(\mathbb{C})$ and $H(\Delta)$ are equipped with the algebra structure afforded by pointwise multiplication, the isomorphism is also a homomorphism.

Certain classes of Cauchy convolution algebras have particularly regular properties. A sequence space is said to be perfect if

$$\lambda = \lambda^{\times\times}. \tag{3.22}$$

As usual, we assume that λ carries its normal topology. It is said to be of type h (Dubin and Hennings [1-2]) if

$$a \in \lambda \quad \Rightarrow \quad (e^n a_n)_{\mathbb{N}} \in \lambda. \tag{3.23}$$

Let λ be perfect, type h, be a subalgebra of h, and have a jointly continuous product. The first two conditions imply that both λ and its strong dual are complete, nuclear and reflexive, and the strong dual topology on the dual is equivalent to its normal topology. ■

The most familiar class of topological algebras are C^*–algebras and W^*–algebras. In view of what we have said before, we shall only make a few remarks about these types.

3.10 Definition (a) A C^*–algebra is a B^*–algebra for which the norm satisfies

$$\|x^* x\| = \|x\|^2 \tag{3.24}$$

as well as equations (3.13.a,c).

(b) A W^*–algebra is a C^*–algebra $\mathcal{A}$ for which there exists a Banach space $\mathcal{M}$ whose strong dual is $\mathcal{M}' = \mathcal{A}$.

(c) A complete topological *–algebra whose topology is defined by submultiplicative seminorms (p_α) satisfying

$$p_\alpha(x^* x) = p_\alpha(x)^2 \tag{3.25}$$

is known as a b^*–algebra. Seminorms of this type are known as C^*-seminorms. ■

3.11 Remarks (a) Every W^*–algebra is *- isomorphic to a weakly closed *-symmetric algebra of bounded operators on some Hilbert space. Similarly, every C^*–algebra is *-isomorphic to a uniformly closed *- symmetric algebra of bounded operators on some Hilbert space.

(b) Define the commutant $\mathcal{M}'$ of a set $\mathcal{M}$ of bounded operators on a Hilbert space as the set of all bounded operators which commute with all of $\mathcal{M}$. Similarly, the bicommutant $\mathcal{M}''$ is the commutant of $\mathcal{M}'$.

Von Neumann has shown that a *-symmetric unital algebra $\mathcal{M}$ of bounded operators on a Hilbert space is weakly closed iff $\mathcal{M} = \mathcal{M}'$.

(c) In the Arens-Michaels decomposition of a b^*–algebra, the components may be taken to be C^*-algebras. Another name for these algebras is locally C^*–algebras (Inoue [1]). It is worth noting that a C^*-seminorm is automatically submultiplicative (Sebestyen [1]). ■

Extensive treatments of the above material may be found in the texts cited above. For the record we note the following miscellaneous examples.

3.12 Examples (a) The set of all compact operators on a Hilbert space is a C^*–algebra when equipped with the uniform topology obtained from the operator norm.

(b) Let $\mathcal{A}$ be an abelian unital C^*–algebra. Then it is isomorphic as a C^*–algebra to $\mathcal{C}(K)$, where K is the compact Hausdorff space of maximal ideals of $\mathcal{A}$. If $\mathcal{A}$ is nonunital, it is similarly isomorphic to the space $\mathcal{C}_0(X)$ of all functions vanishing at infinity, where now the spectrum space X is a locally compact Hausdorff space. Both $\mathcal{C}(K)$ and $\mathcal{C}_0(X)$ are equipped with the supremum norm.

(c) The space $\mathcal{L}(\mathcal{H})$ of all bounded operators on the separable Hilbert space $\mathcal{H}$ is a W^*–algebra with the uniform topology. Its pre-dual Banach space is the space of all trace class operators on $\mathcal{H}$ with the trace norm.

For any C^*–algebra $\mathcal{A}$, its second topological dual is a W^*–algebra, and may be identified with the weak closure of the universal representation of $\mathcal{A}$.

(d) If $\mathcal{A}$ is an abelian W^*–algebra it is W^*-isomorphic to

$$\mathcal{A} \cong L^\infty(X, \mu), \tag{3.26}$$

where (X, μ) is a direct sum of finite measure spaces with positive Radon measures.

(e) The reader will recall the C^*–algebra of the *ccr* constructed in Proposition [2.27], denoted $\mathtt{A}$ there. Its Schrödinger representation, $\mathtt{A}_S$, has weak closure

$$\mathtt{A}_S'' = \mathcal{L}\left(L^2\left(\mathbb{R}^d\right)\right), \tag{3.27}$$

the W^*–algebra of all bounded operators. ■

An element x of an algebra $\mathcal{A}$ is said to be quasi-invertible if there exists a $y \in \mathcal{A}$ such that

$$x + y + xy = 0. \tag{3.28}$$

Notice that if $\mathcal{A}$ is unital, x is quasi-invertible if and only if $e + x$ is invertible.

A locally convex algebra $\mathcal{A}$ is said to be a Q-algebra if the set of quasi-invertible elements is open. It is well known that all Banach algebras are Q-algebras; indeed, it is often precisely the Q property that enables many of the standard results of Banach algebra theory to go through. Hence, those results can usually be generalized to Q-algebras.

A spectral theory for locally convex algebras can be introduced in much the same way as for normed algebras, and a spectral radius function ν can be defined (Allen [1], Mallios [1], Michael [1]). In contrast with the spectral theory for normed algebras, $\nu(x)$ can be infinite for some elements of $\mathcal{A}$. Without proving them, we note the following results.

3.13 Proposition Let $\mathcal{A}$ be an algebra. The spectrum $\sigma(x)$ of an element $x \in \mathcal{A}$ is the set

$$\{\lambda \in \mathbb{C}^* : -x/\lambda \,\text{is not quasi-invertible}\}, \tag{3.29.a}$$

together with 0 if either $\mathcal{A}$ is nonunital or x is not invertible. This coincides with the usual definition if the algebra is unital.

The spectral radius $\nu(x)$ of x is defined to be the set

$$\sup\{\,|\lambda| : \lambda \in \sigma(x)\,\} \tag{3.29.b}$$

when $\sigma(x)$ is nonempty, and $-\infty$ when it is.

If $\mathcal{A}$ is a complete lmc-algebra, then Michael [1] has shown that $\sigma(x)$ is always nonempty, and

$$\nu(x) = \sup_p \left(\lim_{n\to\infty} p(x^n)^{1/n}\right), \qquad x \in \mathcal{A}. \tag{3.29.c}$$

The supremum is to be taken over all continuous seminorms on $\mathcal{A}$. Moreover, he showed that $\mathcal{A}$ is a Q-algebra if and only if the set

$$\mathcal{N} = \{\, x \in \mathcal{A} : \nu(x) < 1\,\}$$

is a neighbourhood of 0. ■

One result more should be noted, as it indicates that the Q property is very strong, and that Q-algebras are comparatively rare. For proofs, see Fragoulopoulou [1], Phillips [1].

3.14 Proposition Any Q b^*–algebra is a C^*–algebra. ■

In the category of locally convex spaces, the morphisms are the continuous linear maps between spaces. The study of the spaces of such maps is very important in the theory, particularly for tensor products and distributions. As the space of all continuous linear maps from a *tvs* to itself is an algebra, it is evidently worth considering.

As usual, let $\mathcal{L}_b(E,F)$ be the space of continuous linear maps from E into F, equipped with the strong topology of bounded convergence. Recall the convention that if $E = F$, we write $\mathcal{L}_b(E)$.

3.15 Theorem (a) If E is bornological and F is complete, then $\mathcal{L}_b(E,F)$ is complete. This will certainly be the case when E and F are nuclear Fréchet spaces.

(b) Let E be a nuclear Fréchet space. Then $\mathcal{L}_b(E)$ is a complete nuclear locally convex algebra.

Proof (a) is standard *tvs* material. Now consider (b). The linear structure is also standard, since

$$\mathcal{L}_b(E) \cong E \widehat{\bigotimes} E'. \tag{3.30}$$

We need only prove that the product is separately continuous to prove the theorem.

Let p be any continuous seminorm on E and V be any bounded subset. For any a, $b \in \mathcal{L}_b(E)$ we note first that

$$p_V(ab) = p_{bV}(a); \tag{3.31.a}$$

and as bV is bounded, p_{bV} is one of the seminorms defining the topology. Hence left multiplication is continuous.

With the same notation, let $q = p \circ a$. Then q is a seminorm. As the composition of continuous maps it is continuous, so

$$p_V(ab) = q_V(b) \tag{3.31.b}$$

shows that right multiplication is continuous, and we are done. ■

Three things are worth noting. First, $\mathcal{L}_b(E)$ is neither a Fréchet nor a DF-space when E is infinite dimensional. Second, when E is a Hilbert space, the bounded topology just considered coincides with the usual operator norm topology. Third, when E is n-dimensional, $\mathcal{L}_b(E)$ is the set of all $n \times n$ matrices.

3.3 STATES, REPRESENTATIONS AND ORDER

Consider a $*$–algebra . The product and involution together allow the construction of elements of the form a^*a and sums of these. It is to be expected that such elements have properties similar to positive numbers as elements of $\mathbb{C}$. Turning from $\mathbb{C}$ to matrices, there is a second natural notion of positivity besides sums of squares, namely matrices for which

$$\langle x, Ax \rangle \geq 0$$

for all vectors x. The extension of this second sort of positivity turns out to be the most useful one for the algebra of observables. For the convenience of the reader, we shall now write down some results of interest to us from the theory of ordered topological vector spaces. This is followed by some illustrative examples. Standard references are Peressini [1] and Schaeffer [1].

All of the complex vector spaces which appear in the text have an underlying real vector space. This is obtained by restricting scalar multiplication to the real field. Order properties refer to real vector spaces. With this in mind, all spaces in this section will be real unless otherwise noted.

3.16 Definition A nonempty convex subset K of a vector space E is a *wedge* if

$(i\ )$ $$K + K \subset K,$$

(*ii*) $\lambda K \subset K$ for all positive λ.

If K is also *proper*, meaning

(*iii*) $$K \bigcap -K = \{0\},$$

it is said to be a *cone*.

A cone (wedge) defines an *order (pre–order) relation* on E by setting

$$x \leq y \qquad \text{if} \qquad y - x \in K. \tag{3.32}$$

If $x \in K$, then $x \geq 0$, and so elements of K are said to be *positive*. K is known as the *positive cone (wedge)*. As E may have more than one positive cone, a more precise notation is to refer to the pair (E, K) as the ordered vector space in question. This will not be necessary here, and E and K will retain a fixed significance until further notice. ■

When considering a complex algebra, it is usual only to consider wedges K which consist of hermitian elements. The complex algebra $\mathcal{A}$ is then said to have a particular property with respect to the wedge K if and only if the real vector space $\mathcal{A}_h$ of hermitian elements has that property with respect to K.

3.17 Definition (a) K is *generating* if

$$E = K - K. \tag{3.33}$$

(b) Sets in E of the form

$$[\![x, y]\!] = \{ z \in E : x \leq z \leq y \} \tag{3.34}$$

are known as *order intervals*.

(c) A set $B \subset E$ is *order bounded* if it is contained in some order interval.

(d) An element $x \in E$ is an *order unit* if the order interval $[\![-x, x]\!]$ is absorbing.

(e) A linear map between ordered vector spaces is positive if it maps the domain positive cone into the range positive cone.

(f) A linear map between ordered vector spaces is is said to be order bounded if it maps order bounded sets to order bounded sets. ■

In the general case, the relation between topology and order is rather weak. It is considerably strengthened by requiring equation (3.35) below to hold.

3.18 Definition Let $E[t]$ be a *lcs* ordered by the cone K. We shall say that E is an ordered locally convex space, or *olcs*. (This is Peressini's usage [1]; it differs from that of Schaeffer [1] and Bourbaki [1].)

The cone K is normal if there is a generating family Γ of seminorms for t such that

$$p(x) \leq p(x+y) \qquad \text{for all } x, y \in K,\ p \in \Gamma. \tag{3.35}$$

■

Just how strong normality is can be seen from the fact that it guarantees the propriety of the wedge.

3.19 Proposition (a) A positive wedge in a *lcs* which satisfies equation (3.35) is necessarily a cone.

(b) If the positive cone in the ordered locally convex space E is normal, every order bounded set is bounded in the original topology t.

(c) The closure of a normal cone in an ordered locally convex space is a normal cone.

(d) If M is a subspace of the ordered locally convex space E and K is normal, then M is an ordered locally convex space with normal cone $M \bigcap K$.

(e) If K is normal and has a non-empty interior, then $E[t]$ is normable. ■

Next we consider the relation between order and duality. Positivity of functionals is necessary for their physical interpretability.

3.20 Definition (a) Let E be an ordered locally convex space with cone K. The subset of E' given by

$$K' = \{\, T \in E' : T(x) \geq 0, \qquad \text{all } x \in K \,\}. \tag{3.36}$$

is the *dual wedge*. If it is proper, it is known as the dual cone. Elements of K' are known as *continuous positive linear functionals*.

(b) Let K^* denote the set of all positive linear functionals. That is, elements of E^* which are positive on K. The *order dual* of E is the linear subspace

$$E^*_+ = K^* - K^* \tag{3.37}$$

of the algebraic dual E^*.

E is *regularly ordered* if E^*_+ separates points of E. If E is regularly ordered, so is any subspace. ■

Every Radon measure on a locally compact Hausdorff space can be written as the difference of two positive Radon measures. This is equivalent to the classical Hahn–Jordan decomposition. Ultimately, this result depends on the fact that the positive Radon measures constitute a normal cone. This is generally true.

3.21 Proposition (a) The dual wedge is a cone if and only if $K-K$ is $\sigma(E,E')$ dense in E.

(b) If K is a normal cone, K' is generating. That is, every $T \in E'$ is the difference of two positive functionals. ■

If a cone is normal, in many cases this characterizes its dual cone, and vice versa. This true, eg, for the cone dual to the positive Radon measures, the cone of positive valued continuous functions of compact support.

3.22 Definition A cone K in an ordered locally convex space E is said to be a *strict b-cone* if

$$\left\{ B\bigcap K - B\bigcap K : \text{every bounded}\, B \subset E \right\}$$

is a total family of bounded subsets.

It is a *b-cone* if

$$\left\{ \overline{B\bigcap K - B\bigcap K} : \text{every bounded}\, B \subset E \right\}$$

is a total family of bounded subsets. ■

Just when this property is dual to normality can be made explicit.

3.23 Proposition (a) If K is normal in $E[t]$, then it is normal for $\sigma(E,E')$.

(b) Suppose $E[t]$ is reflexive, K is closed, and $K-K$ is dense. Then K is normal iff K' is a b-cone in E'_b.

Conversely, K is a b-cone iff K' is normal in E'_b. ■

This next result can be useful on occasion.

3.24 Proposition If E is a regularly ordered vector space, then there is a locally convex topology on E for which K is normal. This is equivalent to the closure of K in the finest locally convex topology being a cone. ■

An order relation can be used to determine, in a certain sense, a topology. As Schaeffer [1] points out, this order topology is equivalent to the original topology for many of the ordered vector spaces occurring in practice.

3.25 Definition The *order topology* r on an ordered vector space is the finest locally convex topology, not necessarily Hausdorff, for which every order bounded set is r-bounded. ■

The relation between the order topology and the original topology often hinges on this next result.

3.26 Proposition Let E be a regularly ordered vector space. Then r is bornological.

Suppose E has the decomposition property

$$[\![0, x + y]\!] = [\![0, x]\!] + [\![0, y]\!], \qquad \text{all}\, x, y \in K.$$

Then the order topology is the finest locally convex topology for which K is normal. It is also the Mackey topology, and the space of all order bounded linear functionals coincides with E'. ■

This next result will be used in the proof of the equivalence between the order and original topologies for the algebra of observables,

3.27 Proposition Let $H \subset K$ be such that for each $x \in K$ there is an $h \in H$ and $\lambda > 0$ such that $x \leq \lambda h$.

Suppose E is regularly ordered. Define p_h to be the gauge of the order interval $[\![-h, h]\!]$. This is a norm on

$$E_h = \bigcup_{n=1}^{\infty} n[\![-h, h]\!], \qquad h \in H, \tag{3.38}$$

and the order topology on E is the inductive topology with respect to the family $\{\, E_h[p_h] : h \in H \,\}$. ■

For a *-algebra we can consider the sums of squares a^*a as constituting a positive wedge, as already noted. In general, this wedge may not be a cone.

3.28 Definition For a *-algebra $\mathcal{A}$ we define the algebraic positive wedge to be the subset

$$P(\mathcal{A}) = \left\{ \sum\nolimits_{n=1}^{N} x_n^* x_n : x_n \in \mathcal{A},\ N < \infty \right\}. \tag{3.39}$$

If the algebraic wedge is a cone, and if the algebra has an identity e, then $P(\mathcal{A})$ is generating. For we may write any $a \in \mathcal{A}_h$ as

$$a = (e + a)^2/4 \; - \; (e - a)^2/4 \tag{3.40.a}$$

$$= a_+ - a_-, \qquad a_\pm \in P(\mathcal{A}). \tag{3.40.b}$$

In the usual notation for generating cones, we write

$$\mathcal{A}_h = P(\mathcal{A}) - P(\mathcal{A}). \tag{3.40.c}$$

■

For a topological *-algebra with a positive cone, there are three distinct structures delineated above: an algebra, a topological vector space, and an ordered vector space. The interaction between them is what gives the subject its characteristic nature.

The reader should note that some authors refer to a wedge as a cone, and to a cone as a proper cone.

3.29 Examples (a) For any C^*–algebra , the algebraic positive cone $\mathcal{P}$ is proper and equal to its closure. Moreover, we have the remarkable result that every positive element is of the form x^*x, so that

$$\mathcal{P} = \{\, x^*x : x \in \mathcal{A} \,\}.$$

For a proof, see Bratteli and Robinson [1], 2.2.2 of Volume 1. Taking projective limits, we see that the same is true for b^*–algebras (Fragoulopoulou [2]).

(b) Peressini gives the following examples of normal cones. (1) The cone of vectors in $\mathbb{R}^n$ with all components non negative. (2) The cone of sequences in ϕ and ω with non negative components. (3) The non negative valued functions on a compact Hausdorff space, which are either bounded or continuous. These spaces are to have the sup norm topology. (4) The non negative valued functions, μ-almost everywhere, in $L^p(X, \mu)$ for an arbitrary measure space. (5) The cones dual to these are strict-b. (6) The cone of non negative valued functions in $\mathcal{D}(\mathbb{R}^d)$ is strict-b and not normal. The dual cone of distributions is then normal and not strict-b.

(c) Going back to Cauchy convolution algebras, [3.9], let λ be perfect, type h, be a subalgebra of h, and have a jointly continuous product. Under these four conditions, the positive cone $\mathcal{P}$ of λ is a proper strict-b cone, as is its closure. Conditions are known for the cone to be normal, but they are not sufficiently practical to determine whether or not this is true for most of the spaces λ. It is well known that the cone $\mathcal{P}$ is normal for $\lambda = \phi$, but less well known that it is not for the space h (Dubin and Hennings [1,2]). ■

In the theory of locally convex spaces the concept of duality is of critical importance. In the theory of topological groups, unitary representations are of similar importance. For topological algebras these notions have been known to be related. This is the topic we shall discuss in this section. It differs from the theory for normed algebras by virtue of nontrivial domain questions. For more details we refer the reader to the work of Powers [1] and Gudder and Scruggs [1].

3.30 Definition Let $\mathcal{A}$ be a locally convex *–algebra, and $\mathcal{A}'$ its dual. An involution is introduced into $\mathcal{A}'$ by

$$T^*(a) = \overline{T(a^*)}. \tag{3.41.a}$$

A functional is said to be hermitian if

$$T^* = T, \tag{3.41.b}$$

and the set of all hermitian functionals is written as $\mathcal{A}'_h$.

Suppose that K is a cone in $\mathcal{A}$ containing the algebraic wedge $P(\mathcal{A})$. A functional is said to be positive with respect to K if

$$T(a) \geq 0, \qquad \forall a \in K. \tag{3.42.a}$$

If $\mathcal{A}$ is unital, then a positive functional is said to be a state if

$$T(e) = 1. \tag{3.42.b}$$

The set of states will be written as S.

A state T will be said to be faithful if $T(a^*a) = 0$ implies that $a = 0$. The left kernel of a state T is the left ideal

$$L_T = \{ a \in \mathcal{A} : T(a^*a) = 0 \}. \tag{3.42.c}$$

The set of positive functionals will be written as $\mathcal{A}'_+$. ■

The reader will note that $\mathcal{A}'_+$ is none other than the dual wedge K'. One often writes K as $\mathcal{A}_+$. The symbols $\mathcal{P}(\mathcal{A})$ and $\mathcal{P}(\mathcal{A})'$ are reserved for the algebraic wedge and its dual.

For topological algebras which are not locally convex, it can happen that the set of continuous functionals is trivial. For locally convex algebras this cannot happen, as a consequence of the Hahn–Banach theorem. This is the only case we shall consider.

Just as for the algebra itself, the existence of an involution implies that equation (3.4) holds for the dual:

$$\mathcal{A}' = \mathcal{A}'_h + i\,\mathcal{A}'_h. \tag{3.43}$$

Then $\mathcal{A}'_h$ is a real ordered topological vector space, the real continuous dual of $\mathcal{A}_h$. The condition that the dual cone is generating is too strong, in general. It may often be replaced by the weaker condition that $\mathcal{A}'_+ - \mathcal{A}'_+$ is dense in $\mathcal{A}'_h$.

The connecting link to representations will be the Cauchy–Schwarz inequality.

3.31 Proposition Every positive functional satisfies the Cauchy–Schwarz inequality

$$|T(a^*b)|^2 \le T(a^*a)\,T(b^*b). \tag{3.44}$$

Proof This is shown as in the normed case, by minimizing

$$f(x) = T\left[(a+\lambda x b)^*(a+\lambda x b)\right], \qquad (x \in \mathbb{R}),$$

where λ is a complex number of unit modulus such that

$$\lambda\, T(a^*b) = |T(a^*b)|.$$

■

We now introduce a few of the sorts of representations associated with *–algebras. There are more, which we shall not need, and the relations between them are complicated.

3.32 Definition Let $\mathcal{A}$ be a *–algebra . A *–representation of $\mathcal{A}$ is a pair (π, D) where D is a dense subspace of a Hilbert space $\mathcal{H}$, and

$$\pi : \mathcal{A} \to L(D) \tag{3.45.a}$$

is an algebra homomorphism into the linear operators on D such that

$$\langle x, \pi(a)y\rangle = \langle \pi(a^*)x, y\rangle, \qquad a \in \mathcal{A};\ x, y \in D. \tag{3.45.b}$$

Note that every operator $\pi(a)$ is closable in $\mathcal{H}$, and that $\pi(a^*) \subseteq \pi(a)^*$.

A *–representation (π_1, D_1) is said to be an extension of (π, D) if $D \subseteq D_1$ and $\pi(a) \subseteq \pi_1(a)$ for all $a \in \mathcal{A}$.

We indicate by t the graph topology on D determined by the set $\pi(\mathcal{A})$. Each represented operator is continuous, *ie* , $\pi(\mathcal{A})$ is a subset of $\mathcal{L}(D[t])$.

If $\mathcal{A}$ is a locally convex algebra, the *–representation will be said to be continuous if π is continuous from $\mathcal{A}$ to $\mathcal{L}_b(D[t])$. The *–representation is said to be closed if $D[t]$ is complete. Any *–representation has a unique minimal closed extension, given by

$$\overline{D} = \bigcap\nolimits_{\mathcal{A}} D\left(\overline{\pi(a)}\right), \quad \overline{\pi}(a)x = \overline{\pi(a)}x. \tag{3.46}$$

The adjoint of a *–representation (π, D) is the pair (π^*, D^*) defined by

$$D^* = \bigcap_{\mathcal{A}} D\left(\pi(a)^*\right), \quad \pi^*(a)x = \pi(a^*)^* x. \tag{3.47}$$

The *–representation (π, D) is said to be essentially self adjoint if its adjoint is a *–representation. It is said to be self adjoint if it coincides with its adjoint. The *–representation (π, D) is said to be cyclic if there exists a nonzero vector $w \in D$ such that $\pi(\mathcal{A})w$ is dense in $\mathcal{H}$. The vector w is then said to be a cyclic vector.

The *–representation is said to be strongly cyclic if $\pi(\mathcal{A})w$ is dense in $D[t]$, in which case w is said to be strongly cyclic. If $\pi(\mathcal{A})w = D$, the *–representation is said to be ultracyclic, and w an ultracyclic vector.

Two *–representations (π_1, D_1) and (π_2, D_2) are equivalent if there exists a unitary operator V from $\mathcal{H}_1$ onto $\mathcal{H}_2$ such that

$$V D_1 = D_2, \qquad \text{and} \qquad V\pi_1(a) = \pi_2(a)V \tag{3.48}$$

for all $a \in \mathcal{A}$.

A vector $v \in D$ is said to be separating if $\pi(a)v = 0$ implies that $a = 0$. ■

Proofs of the following results can be found in the two references above. The Gel'fand, Naimark and Segal representation (GNS) furnishes the connection between states and representations.

3.33 Proposition (a) Let (π, D) be a *–representation of $\mathcal{A}$. Then

$$\pi \subset \overline{\pi} \subset \pi^{**} \subset \pi^*. \tag{3.49}$$

Every *–representation extending π is a restriction of its adjoint, which latter need not be a *–representation.

The closure of a strongly cyclic *-representation is a closed strongly cyclic *-representation.

(b) Consider the following conditions for a self adjoint representation (π, D): (1) Define the bounded weak commutant as

$$\pi'_w = \left\{ a \in \mathcal{L}(\mathcal{H}) : \langle a\, x,\, b y\rangle = \langle b^+ x,\, a^* y\rangle, \quad x, y \in D,\, b \in \mathcal{A} \right\}. \tag{3.50}$$

Then

$$\pi'_w = \mathbb{C}\, I \tag{3.51}$$

is scalar. This will be known as algebraic irreducibility.

(2) The only t-complete subspaces of D which are invariant under $\pi(\mathcal{A})$ are $\{0\}$ and D.

(3) The only subspaces of D which are invariant under $\pi(\mathcal{A})$ and such that π restricted to them is self adjoint, are $\{0\}$ and D.

(4) Every nonzero vector in D is strongly cyclic.

(5) Every nonzero vector in D is cyclic.

Then

$$\begin{array}{ccccc} (3) & \Leftrightarrow & (1) & \Leftarrow & (2) \\ \Uparrow & & & & \Updownarrow \\ (5) & & \Longleftarrow & & (4) \end{array}$$

(c) Let T be a state on a unital *-algebra $\mathcal{A}$. Let $a \to [a]_T$ indicate the projection from $\mathcal{A}$ into its equivalence class in the linear space $D_0 = \mathcal{A}/L_T$. Equip D_0 with the inner product

$$\langle [a]_T, [b]_T \rangle = T(a^* b). \tag{3.52}$$

Let π_0 be the *–representation defined on D_0 by

$$\pi_0(a)\,[b]_T = [ab]_T \tag{3.53}$$

and let $w_T = [e]_T$.

The closure of (π_0, D_0) is a strongly cyclic closed *–representation, with strongly cyclic unit vector w_T. We write (π_T, D_T, w_T) for this closure. Then

$$\langle [a]_T, \pi_T(c)\,[b]_T \rangle = T(a^* c b) \tag{3.54}$$

for all a, b, $c \in \mathcal{A}$. This, the GNS representation, is defined up to unitary equivalence. Note that some authors define the GNS representation to be (π_0, D_0), before closure.

The GNS representation is algebraically irreducible if and only if the state T is extreme in the set of states. Such states will also be known as pure. For brevity we often drop the T subscript if it will cause no confusion. ∎

For illustrative purposes, and without proof, we present a few examples, taken from Powers [1] and Mallios [1].

3.34 Examples (1) Let $\mathcal{A}_n$ be the free commutative algebra on n commuting generators. Elements of $\mathcal{A}_n$ are then polynomials in the generators. The following is a self adjoint representation. Let m be a regular Borel measure on $\mathbb{R}^n$, and the Hilbert space of the representation is $L^2(\mathbb{R}^n, m)$. For any polynomial p in n variables, let $P = p(a_1, \ldots, a_n)$ be an element of $\mathcal{A}_n$.

The domain is

$$D = \left\{ f \in L^2(\mathbb{R}^n, m) : \int |p(\xi) f(\xi)\, dm(\xi)|^2 < \infty, \forall p \right\}, \tag{3.55.a}$$

and the homomorphism is

$$[\pi(P)f](\xi) = p(\xi)f(\xi), \qquad (\xi \in \mathbb{R}^n). \tag{3.55.b}$$

(2) Here is a self adjoint representation of $\mathcal{A}_2$ which satisfies the algebraic irreducibility condition above. Let Ω be the square of side π in $\mathbb{R}^2$, centred at the origin; the representation Hilbert space is $L^2(\Omega)$, with Lebesgue measure. The domain is

$$D = \left\{ f \in \mathcal{C}^\infty(\Omega) : \begin{Bmatrix} \partial_1^n f(-\pi, y) = e^{iy} \partial_1^n f(\pi, y) \\ \partial_2^n f(x, -\pi) = \partial_2^n f(x, \pi) \end{Bmatrix} \quad n \geq 0 \right\}, \tag{3.56.a}$$

and the homomorphism is

$$\pi(a_1)f = -i\partial_1 f \qquad \text{and} \qquad \pi(a_2)f = -i\partial_2 f. \tag{3.56.b}$$

(3) The existence of an invariant subspace does not imply that the projection onto its closure is in the weak commutant, as is the case for bounded *-representations of *-algebras. To see this, consider $\mathcal{A}_1$ represented on $L^2(\mathbb{R})$ as follows. Let

$$D = \left\{ f \in \mathcal{C}^\infty : f^{(n)} \in L^2(\mathbb{R}), n \geq 0 \right\}, \tag{3.57.a}$$

and

$$\pi(a_1)f = -if'. \tag{3.57.b}$$

Consider the subspace

$$M = \{ f \in \mathcal{C}^\infty : f([0,1]) = 0 \}. \tag{3.58}$$

This subspace is invariant under $\pi(\mathcal{A}_1)$, but the projection P onto its closure is not an element of the weak commutant.

(4) Let $\mathcal{A}$ be abelian. Let P be a positive polynomial in hermitian elements of $\mathcal{A}$. A state T is said to be strongly positive if $T(P)$ is positive for all such P. A *–representation is said to be strongly positive if then $\pi(P)$ is a positive operator.

By an example of Gel'fand and Vilenkin [1], positivity does not imply strong positivity. Let q be the famous Hilbert polynomial in two variables, which is of sixth degree, takes strictly positive values on $\mathbb{R}^2$, and is not a sum of squares. They exhibit a state T on $\mathcal{A}_2$ for which $T(q(a_1, a_2))$ is negative.

This is connected to the moment problem. For if T is a state on $\mathcal{A}_n$, a necessary and sufficient condition for there to exist a regular Borel measure m on $\mathbb{R}^n$ such that

$$T\left(p(a_1, \ldots, a_n)\right) = \int p(\xi)\, dm(\xi) \tag{3.59}$$

for all positive polynomials, is that T is strongly positive (Choquet [1]).

Strong positivity together with self adjointness is extremely restrictive. Let π be a strongly cyclic self adjoint *–representation of an abelian *-algebra $\mathcal{A}$. Let w be a normalized strongly cyclic vector for the representation, and let T be the state it defines:

$$T(a) = \langle w, \pi(a)w \rangle. \tag{3.60}$$

Then the following four conditions are equivalent

(i) $$\pi(a)^* = \overline{\pi(a)}, \qquad \forall a \in \mathcal{A}_h;$$

(ii) $$\pi(a)^* = \overline{\pi(a^*)}, \qquad \forall a \in \mathcal{A};$$

(iii) π'_w is abelian;

(iv) T is strongly positive.

(5) Let π be an algebraically irreducible representation of $\mathcal{A}$ on a domain D. Suppose that v, w are vectors in D such that the vector states they define coincide:

$$\langle v, \pi(a)v \rangle = \langle w, \pi(a)w \rangle, \qquad (a \in \mathcal{A}). \tag{3.61}$$

Then

$$v = e^{i\theta} w, \tag{3.62}$$

for some phase angle θ.

(6) A state which satisfies the multiplicative condition

$$T(ab) = T(a)T(b) \tag{3.63}$$

is known as a character. The GNS representation arising from a state is one dimensional if and only if the state is a character. As the weak commutant is necessarily scalar, characters are pure states. But example (2) above shows that, in general, *not all pure states are characters.* In that example, the representation was infinite dimensional, and this is general: pure states are either characters or give rise to infinite dimensional representations. For normed algebras, the pure states are always characters.
■

For any abelian C^*-algebra $\mathcal{A}$, the pure states are in one to one correspondence with the maximal closed left ideals. The pure states form a space called the spectrum, Ξ. With an appropriate topology on Ξ there is a C^*-isomorphism between $\mathcal{A}$ and $\mathcal{C}_0(\Xi)$.

This well known theory has only partial analogues for general locally convex algebras. For an elaboration of the theory we refer to Mallios [1]. Here are a few results, without proof.

3.35 Examples (1) Let $\mathcal{A}$ be a unital abelian algebra, and I a maximal two sided ideal. Then $\mathcal{A}/I$ is an abelian division algebra over $\mathbb{C}$. Note that there exist non trivial complex abelian division algebras, for example the rational polynomials $\mathbb{C}(X)$ in one indeterminate.

(2) Let $\mathcal{A}$ be a unital abelian locally convex Q-algebra. Let I be a maximal two sided ideal. Then I is closed and $\mathcal{A}/I$ is isomorphic to $\mathbb{C}$.

(3) Let $\mathcal{A}$ be the unital abelian algebra $\mathcal{C}^\infty(\mathbb{R})$ be equipped with the topology determined by the seminorms

$$f \to \sup_{k \leq n} \sup_{x \in K} \left| f^{(k)}(x) \right|, \tag{3.64}$$

for $n \in \mathbb{N}$ and compact K. With this topology, $\mathcal{A}$ is a Fréchet lmc algebra.

The set of characters of $\mathcal{A}$ is in one to one correspondence with its closed maximal two sided ideals, $\mathcal{M}$, the continuous spectrum of the algebra. The evaluation map

$$\delta : \mathbb{R} \to \mathcal{A}'[\sigma(\mathcal{A}', \mathcal{A})] \tag{3.65}$$

is a homeomorphism whose range is contained in $\mathcal{M}$. If $\mathbb{R}$ is replaced by a compact subset, the range is onto the continuous spectrum. ■

This ends our preliminary discussion of topological algebras. The next chapter continues with an analysis of the algebra of observables for the canonical commutation relations.

4. THE ALGEBRA OF OBSERVABLES

4.1 THE ALGEBRA $\mathcal{L}^{+}\left(\mathcal{W}_{\vec{N},\vec{t}}\right)$

In the previous chapter we introduced a number of concepts relating to, and examples of, topological algebras. Now we return to the consideration of elementary quantum systems, as defined in Axiom 0. In Axiom 1 we determined the relevant spaces of wave functions. Consulting that axiom and equation (2.78) , we recall that

$$\mathcal{W}_{(\vec{N},\vec{t})} = \widehat{\bigotimes}_{j=1}^{n} \mathcal{W}_{(N_j,t_j)}[\nu_j] \tag{4.1.a}$$

$$= \mathcal{C}^{\infty}\left(\widehat{\bigotimes}_{j=1}^{n} \mathrm{M}_{(N_j,t_j)}\right) \tag{4.1.b}$$

$$= \mathcal{C}^{\infty}\left(\mathrm{M}_{(\vec{N},\vec{t})}\right) \tag{4.1.c}$$

is the space of wave functions for the system $\Sigma_{(\vec{N},\vec{t})}$ consisting of N_j particles of type t_j, $j = 1, \ldots, n$.

As noted in Chapter 2, when the detailed nature of the system is not important we omit the indices, and write Σ to indicate the system, and $\mathcal{W}$ for the space of wave functions.

We now seek a candidate for the algebra containing all the quantum operators. In order to fix a terminology we shall refer to these operators as *observables*, and the algebra as *the algebra of observables* for the system. We emphasize that this is no more than a convenient courtesy title, and does not imply the physical measurability of any particular observable.

We also intend committing the standard solecism of identifying the mathematical operators with the abstract notion they represent. That is, we treat the philosophical problem of *interpretation* as admitting of a standard solution. For an introduction to the problem of interpretation of physical theories, we refer the reader to Jammer [2], which also contains further references.

Three conditions must certainly be satisfied by our posited algebra of observables, which we denote by $\mathcal{A}$. First, every observable must be a continuous linear operator on the space $\mathcal{W}$ of wave functions. That is,

$$\mathcal{A} \subseteq \mathcal{L}(\mathcal{W}). \tag{4.2}$$

The second requirement is that if $a \in \mathcal{A}$ is an observable, then its Hilbert space adjoint must also be an observable, hence be an element of $\mathcal{A}$. We know that certain important observables are symmetric, the momentum being an example; and it will turn out that symmetry is a necessary condition for physical observability. From the existence of an adjoint we get a notion of positivity, and we shall see later that the whole edifice of measurability is based on certain families of positive operators.

Now it would be mathematically possible to consider an algebra which was only partially stable under the adjoint, but that seems rather too economical. We conclude that we should consider a topological subalgebra of $\mathcal{L}(\mathcal{W})$ which is a topological *–algebra with respect to the involution inherited from the Hilbert space adjoint.

The reader should carefully note the following. Suppose a is an observable. We demand that a be a closable operator on the Hilbert space, and that a^* be a continuous linear map of $\mathcal{W}$ into itself. But the domain of a^* will generally be strictly larger than $\mathcal{W}$, so what we really must consider is the Hilbert space adjoint restricted to the domain $\mathcal{W}$. For our purposes, a precise definition of the adjoint is best given in terms of the dual space $\mathcal{W}'$. Our rather fastidious treatment of the adjoint will be justified when we come to the kernel and trace representations for states.

4.1 The Adjoint For $a \in \mathcal{L}(\mathcal{W})$, let $\tilde{a} \in \mathcal{L}(\mathcal{W}')$ be its transpose. Since the embedding $\mathcal{W} \hookrightarrow \mathcal{W}'$ afforded by equation (2.88) involves identifying a Hilbert space with its dual, it is most natural at this stage to implement this embedding via the continuous injective antilinear map $k : \mathcal{W} \to \mathcal{W}'$, which has dense range, given by the formula

$$[kx, y] = \langle x, y \rangle, \qquad x, y \in \mathcal{W}. \tag{4.3}$$

The crucial point here is that the inner product pairing does, and the dual pairing does not, involve a complex conjugation; k keeps track of the distinction. Note also that we use square brackets for the dual pairing.

It is not always the case that $\tilde{a}kx \in \operatorname{Im} k$ for all $x \in \mathcal{W}$; we say that a is adjointable if this is the case. That is, $a \in \mathcal{L}(\mathcal{W})$ is adjointable if $\tilde{a}kx \in \operatorname{Im} k$ for all $x \in \mathcal{W}$. In this case we define $a^+ \in L(\mathcal{W})$ by setting

$$a^+ x = k^{-1}\tilde{a}kx, \qquad x \in \mathcal{W}. \tag{4.4.a}$$

Clearly a^+ satisfies the equation

$$\langle a^+ x, y \rangle = \langle x, ay \rangle, \qquad x, y \in \mathcal{W}. \tag{4.4.b}$$

We shall prove below that $a^+ \in \mathcal{L}(\mathcal{W})$. For convenience, we shall refer to a^+ as the adjoint of a, if no confusion is likely to occur as a result.

If $a \in \mathcal{L}(\mathcal{W})$ is adjointable, then a is closable, and

$$a^+ = a^*|_{\mathcal{W}}. \tag{4.4.c}$$

It is clear that on the set $\mathcal{L}^+(\mathcal{W})$ of adjointable operators in $\mathcal{L}(\mathcal{W})$, the map $a \to a^+$ is an involution. Then our second requirement is that $\mathcal{A}$ must be a topological *–algebra with respect to this involution.

We note that this notation is consistent with that employed for the raising and lowering operators in Chapter 2. ■

The third constraint is that $\mathcal{A}$ contain all the quantum operators of interest. These include the raising and lowering operators, the angular momenta, the energy, and all polynomials in them. Recalling that $\mathcal{P}$ stands for the algebra of polynomials in the raising and lowering operators, we must have $\mathcal{P} \subseteq \mathcal{A}$. The reader will take care not to confuse this polynomial algebra with the algebraic cone $\mathcal{P}(\mathcal{A})$.

As we are willing to allow as observables operators which may not be directly physically measurable, the most reasonable choice is to take the largest algebra satisfying these conditions.

Axiom 3. The algebra of observables for the quantum system $\Sigma_{(\vec{N},\vec{t})}$ is the set $\mathcal{L}^+\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$ of adjointable operators in $\mathcal{L}\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$. We equip the algebra $\mathcal{L}^+\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$ with the topology of bounded convergence inherited from $\mathcal{L}_b\left(\mathcal{W}_{(\vec{N},\vec{t})}, \left[\mathcal{W}_{(\vec{N},\vec{t})}\right]'_b\right)$ via the antilinear embedding k, and which we denote $\mu_{(\vec{N},\vec{t})}$, or simply μ when the nature of the system is clear. ■

This topology may seem strange, but there are three good reasons for the choice: it will be shown to be the order topology, which, recall, is the finest locally convex topology for which all order intervals are bounded ; it is the finest locally convex topology on $\mathcal{L}^+(\mathcal{W})$ such that the positive cone is normal; and most importantly, it is that topology for which the continuous states are given by density matrices. Its principal disadvantage is that $\mathcal{L}^+(\mathcal{W})[\mu]$ is not complete; as we shall show, its completion is $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$.

As noted above, we have chosen the largest unital *–algebra of continuous operators on the domain $\mathcal{W}$ for the algebra of observables. A unital *-subalgebra of $\mathcal{L}^+(\mathcal{D})$ for a dense subspace $\mathcal{D}$ of a Hilbert space is known as an op*-algebra. This class of algebras has been investigated in some detail, particularly by the Leipzig school, whose results will be used extensively in our presentation. A selection of references is Kürsten [1], Lassner [1–6], Lassner and Lassner [1], Lassner and Timmermann [1], Lassner and Uhlmann [1], G.A.Lassner [1], Schmüdgen [1–5], Tröger [1].

4.2 TOPOLOGICAL PROPERTIES OF THE ALGEBRA $\mathcal{L}^+\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$

In Chapter 2 we showed that the ν-topology on $\mathcal{W}$, determined by the number operator, was equivalent to the graph topology determined by the polynomial algebra $\mathcal{P}$ of the ccr . Now $\mathcal{P}$ is a subset of the algebra of observables $\mathcal{L}^+(\mathcal{W})$, so the graph topology $\mathcal{L}^+(\mathcal{W})$ determines is finer than ν; in fact they are equivalent. Also interesting is the fact that every adjointable operator is automatically continuous. In particular, a^+ is continuous for all $a \in \mathcal{L}^+(\mathcal{W})$, so that $a^+ \in \mathcal{L}^+(\mathcal{W})$. Thus $\mathcal{L}^+(\mathcal{W})$ is closed under the $^+$–operation, and is therefore a *–algebra. We now prove these facts.

4.2 Proposition (a) The graph topology on $\mathcal{W}$ determined by the algebra of observables $\mathcal{L}^+(\mathcal{W})$ is equivalent to the ν- topology.

(b) Any endomorphism a on $\mathcal{W}$ whose adjoint a^+ exists and is also an endomorphism of $\mathcal{W}$ is automatically continuous. Hence

$$L^+(\mathcal{W}) = \mathcal{L}^+(\mathcal{W}).$$

Proof (a) Given an observable a, continuity implies that there exists a positive constant C and an index r such that

$$\|ax\|_0 \;\leq\; K\,\|x\|_r.$$

As the 0-indexed norm is the Hilbert space norm, this shows that the ν-topology is finer than the observable graph topology. Together with the remarks above, we see that they are equivalent.

(b) Let a be an endomorphism such that a^+ is as well. Let $x_n \to x$ be any convergent sequence in $\mathcal{W}$ such that $ax_n \to y$. For any $z \in \mathcal{W}$,

$$\langle z, ax_n\rangle \rightarrow \langle z, y\rangle\,,$$

and

$$\left\langle a^+z, x_n\right\rangle \rightarrow \left\langle a^+z, x\right\rangle.$$

As $\mathcal{W}$ is dense in the Hilbert space, $ax = y$, proving that the graph of a is closed. As $\mathcal{W}$ is a Fréchet space, the closed graph theorem implies that a is continuous. ∎

Our analysis of the space of wave functions has led to rather detailed and complete results. Every wave function can be expressed in terms of a sequence and Hermite functions. The space itself can be obtained entirely through the appropriate number operator.

Unfortunately, such explicit results cannot be obtained for the algebra of observables. This should not be so surprising, for whereas the wave function space is obtained from one operator, the algebra contains many noncommuting operators. Given a general observable, we do not even know exactly what functions of it are also observables. For the position and momentum operators we do happen to have this knowledge, but this is exceptional. Indeed, even the proof that a given class of potentials leads to automorphism groups of the algebra is rather involved.

With this in mind, the sorts of thing we can do are these. We can analyze the consequences of our choice of topology, including the order properties. We can consider a kernel representation for observables. In the next chapter we consider the states on the algebra, and so the work here carries over there. With quantum measurement theory in mind, we shall consider spectral decompositions of observables, and positive maps on the algebra. Finally, we consider the notion of complete sets of commuting observables, Dirac's notion adapted to the framework used here.

First, however, we want to generalize Proposition [2.16] to obtain a total family of bounded subsets for $\mathcal{W}_{(\vec{N},\vec{t})}$. In order to do so, we start by giving the spectral decomposition of the number operator of equation (4.1) . We omit a proof as the result is no more than combining tensor products of spectral decompositions with the symmetry operations. The index calculus in this and the next proposition is rather involved. Unfortunately, there does not seem to be a simpler alternative.

4.3 Lemma (a) We start with a single species, N particles of type t. Introduce the index set

$$I(1,t) = \mathbb{N}^3 \times \{1, 2, \ldots, 2s+1\}.$$

The first three components relate to space, and the fourth relates to spin. Elements of $I(1,t)$ will be denoted

$$\vec{\xi} = (\xi_1, \xi_2, \xi_3, \xi_4).$$

To accommodate the symmetry requirements we introduce the following order relation on $I(1,t)$:

equip $I(1,t)$ with the standard lexicographic order. Explicitly,

$$\vec{\xi} \prec \vec{\zeta} \quad \Leftrightarrow \quad \left\{ \begin{array}{llll} \xi_1 < \zeta_1 & \text{or} & & \\ \xi_1 = \zeta_1, & \xi_2 < \zeta_2 & \text{or} & \\ \xi_1 = \zeta_1, & \xi_2 = \zeta_2, & \xi_3 < \zeta_3 & \text{or} \\ \xi_1 = \zeta_1, & \xi_2 = \zeta_2, & \xi_3 = \zeta_3, & \xi_4 < \zeta_4. \end{array} \right\}$$

If the particle type is Bosonic, the relation on $I(1,t)$ is extended to include equality, and we write

$$\vec{\xi} \preceq \vec{\zeta}$$

in this case. With this order, $I(1,t)$ is totally and well ordered for both Bosons and Fermions.

Next we need an ordered index set for the N particles as a whole. By $I(N,t)$ we shall mean N-tuples

$$\Xi = (\vec{\xi}_1, \vec{\xi}_2, \ldots, \vec{\xi}_N), \qquad \vec{\xi}_j \in I(1,t)$$

with components ordered such that

$$\vec{\xi}_j \prec \vec{\xi}_{j+1}, \qquad j = 1, \ldots, N-1$$

in the Fermionic case, and

$$\vec{\xi}_j \preceq \vec{\xi}_{j+1}, \qquad j = 1, \ldots, N-1$$

in the Bosonic case.

The components are themselves vectors, as above, with

$$\vec{\xi}_j = (\xi_{j,1}, \xi_{j,2}, \xi_{j,3}, \xi_{j,4}).$$

The purpose of these indices is to label an eigenbasis of the (N,t) Hilbert space for the system. In a usual notation, let $\{ w_n : n \in \mathbb{N} \}$ be the one particle Hermite functions and $\{ e_k : k = 1, \ldots, 2s+1 \}$ an orthonormal basis for $\mathbb{C}^{2s+1}$.

For each component $\vec{\xi}_j$ of Ξ we set

$$W_{\vec{\xi}_j} = w_{\xi_{j,1}} \otimes w_{\xi_{j,2}} \otimes w_{\xi_{j,3}} \otimes e_{\xi_{j,4}}. \tag{4.5.a}$$

The required (N,t) orthonormal basis is constructed by taking the tensor product for $j = 1, \ldots, N$ and then using the symmetrizer. That is, we consider the basis

$$\Omega_\Xi = \Lambda_\pm \left[W_{\vec{\xi}_1} \otimes W_{\vec{\xi}_2} \otimes \cdots \otimes W_{\vec{\xi}_N} \right], \tag{4.5.b}$$

By P_Ξ we mean the orthogonal projection operator along Ω_Ξ. These are the spectral projections for the total number operator for the (N,t) case.

The spectral values for the number operator are similarly indexed. To see this, we introduce the integers

$$m_{\vec{\xi}_j} = (\xi_{j,1}+1)(\xi_{j,2}+1)(\xi_{j,3}+1), \tag{4.6.a}$$

where $j = 1, \ldots, N$.

The number operator eigenvalues are obtained from these integers by taking their products, namely

$$m_\Xi = m_{\vec{\xi}_1}\, m_{\vec{\xi}_2} \cdots m_{\vec{\xi}_N}. \tag{4.6.b}$$

Putting things together, the spectral representation for the (N,t) number operator is

$$\mathrm{M}_{(N,t)} = \sum\nolimits_{\Xi \in I(N,t)} m_\Xi\, P_\Xi. \tag{4.6.c}$$

(b) For the general system involving different types of particles as well, the notation is even more complicated, as we must take each different species into account. However, as there is no symmetry constraint between species, only a simple n-fold tensor product occurs.

The general system we are considering consists of N_1 particles of type $t_1, \ldots, N_n$ particles of type t_n, with some fixed finite n. It will be convenient to denote the numbers and types of the system in a vector form, namely $\left(\vec{N}, \vec{t}\right)$.

With this in mind, the ordered index set for the system is simply the product of the index sets for the subsystems. That is,

$$I\left(\vec{N}, \vec{t}\right) = \prod_{k=1}^{n} I(N_k, t_k). \tag{4.7.a}$$

The indices are now written as

$$\boldsymbol{\Xi} = \left(\Xi^1, \ldots, \Xi^n\right),$$

with $\Xi^k \in I(N_k, t_k)$ for the subsystems.

As noted above, the eigenvectors for the number operator are tensor products of the eigenvectors for the subsystems, Ω_{Ξ^k}. We write

$$\Omega_{\boldsymbol{\Xi}} = \Omega_{\Xi^1} \bigotimes \cdots \bigotimes \Omega_{\Xi^n}. \tag{4.7.b}$$

It follows that the spectral projections are tensor products of the projections for the subsystems:

$$P_{\boldsymbol{\Xi}} = \bigotimes_{k=1}^{n} P_{\Xi^k}. \tag{4.7.c}$$

The eigenvalues are products of the subsystem eigenvalues:

$$m_\Xi = \prod_{k=1}^{n} m_{\Xi^k}, \tag{4.7.d}$$

and so the number operator for the general system is

$$\mathrm{M}_{(\vec{N},\vec{t})} = \sum\nolimits_{\Xi \in I(\vec{N},\vec{t})} m_\Xi P_\Xi. \tag{4.7.e}$$

■

The most useful forms for seminorms describing the topology of uniform convergence on bounded subsets clearly require detailed knowledge of bounded subsets. In Proposition [2.16] we described a certain total family B_Γ of bounded subsets of $s^{(d)}$. The construction there was based on the structure of the number operator for $s^{(d)}$, and so we are able to present an analogous construction for $\mathcal{W}_{(\vec{N},\vec{t})}$. As the proof that the construction does in fact lead to a total family is the same as in [2.16], we shall omit it.

4.4 Proposition Define a bijection $\kappa : I\left(\vec{N},\vec{t}\right) \to \mathbb{N}$ such that

$$\kappa\Xi < \kappa\Upsilon \quad \Longleftarrow \quad m_\Xi < m_\Upsilon.$$

We can do this since $\{\,\Xi : m_\Xi = k\,\}$ is a finite set for all $k \in \mathbb{N}$. Now define an ordering on $I\left(\vec{N},\vec{t}\right)$ by setting

$$\Xi \prec \Upsilon \quad \Longleftrightarrow \quad \kappa\Xi < \kappa\Upsilon.$$

Consequently there is a well defined meaning to the convergence of a sequence indexed by $I\left(\vec{N},\vec{t}\right)$, a fact we shall use later.

For each $v \in \mathcal{W}_{(\vec{N},\vec{t})}$ let us write

$$v_\Xi = \langle \Omega_\Xi, P_\Xi v\rangle.$$

Let $\Gamma\left(\vec{N},\vec{t}\right)$ be the subset of $\mathcal{W}_{(\vec{N},\vec{t})}$ given by

$$\Gamma\left(\vec{N},\vec{t}\right) = \left\{ v \in \mathcal{W}_{(\vec{N},\vec{t})} : v_\Xi \geq 0,\ \Xi \prec \Upsilon \Rightarrow v_\Xi \geq v_\Upsilon \right\}.$$

Then for each $v \in \Gamma\left(\vec{N},\vec{t}\right)$,

$$B_v = \left\{ \sum\nolimits_{\Xi \in I(\vec{N},\vec{t})} z_\Xi\, v_\Xi\, \Omega_\Xi : |z_\Xi| \leq 1 \right\} \tag{4.8.a}$$

is an absolutely convex and bounded subset of $\mathcal{W}_{(\vec{N},\vec{t})}$; and

$$\mathrm{B}_{\Gamma(\vec{N},\vec{t})} = \left\{ B_v : v \in \Gamma\left(\vec{N},\vec{t}\right) \right\} \tag{4.8.b}$$

is a total family. ■

As usual, let $\mathcal{L}(E, F)$ be the vector space of all continuous linear maps of the *lcs* E into the *lcs* F. Let $\mathcal{B}$ be the family of all bounded subsets of E, and let Γ be a basis of continuous seminorms of F.

The topology of uniform convergence on bounded subsets for $\mathcal{L}(E, F)$ is that determined by the seminorms

$$p_B(u) = \sup \{ p[u(x)] : x \in B \} . \tag{4.9.a}$$

Here p ranges over Γ and B over $\mathcal{B}$.

From Axiom 3, it follows that the topology $\mu_{(\vec{N},\vec{t})}$ on the algebra of observables $\mathcal{L}^+ \left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$ is determined by the seminorms

$$p_{B,C}(a) = \sup \{ |\langle y, ax\rangle| : x \in B,\ y \in C \} \tag{4.9.b}$$

for all pairs B, C in a total family of bounded subsets.

The obvious inequality

$$p_{B,C} \leq p_{D,D} \qquad \text{with} \qquad D = B \bigcup C$$

shows that the topology may be obtained from the subfamily $(p_{D,D})_D$ along the diagonal, so to speak.

We now improve this result, showing that we can take $x = y$ in equation (4.9.b). The improvement results from a little inequality due to Schmüdgen [1]. We temporarily drop indices for clarity.

4.5 Lemma Let M be an absolutely convex subset of $\mathcal{W}$. If $a = a^+$ is a hermitian observable, then

$$\sup_M |\langle x, ax\rangle| \leq \sup_M |\langle y, ax\rangle| \leq 2 \sup_M |\langle x, ax\rangle| . \tag{4.10.a}$$

If a is not hermitian,

$$\sup_M |\langle x, ax\rangle| \leq \sup_M |\langle y, ax\rangle| \leq 4 \sup_M |\langle x, ax\rangle| . \tag{4.10.b}$$

Proof The first inequality in equation (4.10.a) is obvious. For the second half, choose x, $y \in M$, then a phase factor so that $\langle y, e^{i\theta} ax\rangle$ is real.

As M is absolutely convex, $u_\pm \in M$, where

$$2u_\pm = e^{i\theta} x \pm y .$$

Then

$$\begin{aligned} 4|\langle y, ax\rangle| &= 4\left|\langle y, e^{i\theta} ax\rangle\right| \\ &= 4\,|\langle u_+, au_+\rangle + \langle u_-, au_-\rangle| \\ &\leq 8 \, \sup_M |\langle x, ax\rangle|. \end{aligned}$$

This completes the first part.

For general a, decompose it into hermitian parts,

$$a = a_1 + ia_2.$$

Using equation (4.10.a) and

$$\sup_M |\langle x, a_j x\rangle| \leq \sup_M |\langle x, ax\rangle|,$$

equation (4.10.b) follows immediately, and we are done. ■

We combine these inequalities, the discussion around equation (4.9) , and the bounded sets in the total family $\mathrm{B}_{\Gamma(\vec{N},\vec{t})}$ of Proposition [4.4], to conclude that the following seminorms determine the topology.

4.6 Corollary The topology $\mu_{(\vec{N},\vec{t})}$ on the algebra of observables $\mathcal{L}^+\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$ is determined by the seminorms

$$p_{\mathrm{v}}(a) = \sup\{\,|\langle x, ax\rangle| : x \in B_{\mathrm{v}}\,\}, \tag{4.11}$$

as v varies over $\Gamma\left(\vec{N},\vec{t}\right)$. ■

In view of the next result we shall refer to μ as the *uniform topology* on the algebra of observables.

4.7 Corollary If $\mathcal{H}$ is a Hilbert space, then $\mathcal{L}^+(\mathcal{H})$ is the algebra of all bounded operators, and the topology μ is the usual uniform operator topology. ■

The seminorms of equation (4.11) are convenient for checking the continuity of the involution and the product on the algebra of observables.

4.8 Proposition The algebra of observables, $\mathcal{L}^+\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$, is a topological *–algebra

Proof Evidently

$$p_{\mathbf{v}}(a^+) = p_{\mathbf{v}}(a)$$

for all observables, so the involution is continuous.

Given an observable c and an index $\mathbf{v}$, there is an index $\mathbf{u}$ such that

$$B_{\mathbf{v}} \bigcup c\, B_{\mathbf{v}} \subseteq B_{\mathbf{u}}.$$

Then

$$p_{\mathbf{v}}(a\, c) \leq p_{\mathbf{u}}(a),$$

so right multiplication is continuous. These two results together imply the continuity of left multiplication. ∎

The seminorms of equation (4.11) do not directly emphasize the role of the number operator. To construct a family that does would seem to require not only the use of the total family $\mathrm{B}_{\Gamma(\vec{N},\vec{t})}$, but also the spectral decomposition of the number operator. This can be done, and we start with a result of independent interest, giving the structure of the dual space to $\mathcal{W}$ in terms of the number operator.

4.9 Proposition Let us omit the indices $\left(\vec{N},\vec{t}\right)$ for clarity when we can, and write $\mathcal{W}$ for the space of wave functions, M for the associated number operator, and $\mathcal{H}$ for the system Hilbert space.

For each $\Xi \in I\left(\vec{N},\vec{t}\right)$, let

$$P_{\Xi}\mathcal{H} = \mathcal{H}_{\Xi}$$

be the indicated one dimensional Hilbert space. Then $\mathcal{H}$ can be written as the direct sum of these spaces,

$$\mathcal{H} = \bigoplus_{I(\vec{N},\vec{t})} \mathcal{H}_{\Xi}. \tag{4.12}$$

The space of wave functions, $\mathcal{W}$, contains exactly those elements

$$x = \sum\nolimits_{I(\vec{N},\vec{t})} x_{\Xi}$$

of $\mathcal{H}$ for which the norms

$$q_r(x) = \left(\sum\nolimits_{I(\vec{N},\vec{t})} m_{\Xi}{}^{2r} \|x_{\Xi}\|^2\right)^{1/2} \tag{4.13}$$

are finite, all $r \geq 0$. These norms are equivalent to the M-norms.

The continuous linear functionals $T \in \mathcal{W}'$ are those sequences

$$T = (T_\Xi)_{I(\vec{N},\vec{t})}, \qquad T_\Xi \in \mathcal{H}_\Xi{}'$$

for which the seminorms

$$Q_{\mathrm{v}}(T) = \sum\nolimits_{I(\vec{N},\vec{t})} v_\Xi \, \|T_\Xi\| \tag{4.14}$$

are finite for all $\mathrm{v} \in \Gamma\left(\vec{N}, \vec{t}\right)$. These seminorms determine the strong dual topology.

The dual pairing is the obvious one,

$$T(x) = \sum\nolimits_{I(\vec{N},\vec{t})} T_\Xi\,(x_\Xi)\,. \tag{4.15}$$

Proof The first part is a consequence of the spectral decomposition of the number operator, and the equivalence of the norm systems is straightforward enough to omit the proof.

Clearly a sequence T for which $Q_{\mathrm{v}}(T)$ is finite for all v defines a linear functional on $\mathcal{W}$ via equation (4.15) . Moreover we see that

$$|T(x)| \leq Q_{\mathrm{v}}(T)$$

if $x \in B_{\mathrm{v}}$ and $\mathrm{v} \in \Gamma\left(\vec{N}, \vec{t}\right)$. Thus T maps bounded sets in $\mathcal{W}$ to bounded sets in $\mathbb{C}$. Therefore, since $\mathcal{W}$ is Fréchet , hence bornological, T is continuous.

Conversely, if $T \in \mathcal{W}'$, since $\mathcal{H}_\Xi$ is a one dimensional subspace of $\mathcal{W}$, T must restrict to $T_\Xi \in \mathcal{H}'_\Xi$ for each Ξ.

From the continuity of T on $\mathcal{W}$ we get the bound

$$\|T_\Xi\| \leq C\, m_\Xi{}^r$$

for each Ξ, where r depends only on T and not on the individual components. As

$$\sum m_\Xi{}^r v_\Xi < \infty$$

converges for all r and all v, the characterization of functionals as sequences has been shown.

We must now show that the Q_{v} determine the strong dual topology. Let B_{v} be an arbitrary bounded set from the total family $\mathrm{B}_{\Gamma(\vec{N},\vec{t})}$ of Proposition [4.4] and B°_{v} its polar. Then

$$\begin{aligned}
p_{B^\circ_{\mathrm{v}}}(T) &= \sup\left\{ \left|\sum T_\Xi\,(x_\Xi)\right| : x \in B_{\mathrm{v}} \right\} \\
&\leq \sup\left\{ \sum \|T_\Xi\|\,\|x_\Xi\| : x \in B_{\mathrm{v}} \right\} \\
&\leq \sum v_\Xi\,\|T_\Xi\| \\
&= Q_{\mathrm{v}}(T)\,.
\end{aligned}$$

Conversely, given T_Ξ, since $\mathcal{H}'_\Xi$ is one dimensional, we can choose a complex number α_Ξ, of modulus one, such that

$$v_\Xi \|T_\Xi\| = T_\Xi(\alpha_\Xi v_\Xi \Omega_\Xi).$$

Then

$$\begin{aligned} Q_{\mathrm{v}}(T) &= T\left(\sum \alpha_\Xi v_\Xi \Omega_\Xi\right) \\ &\leq p_{B^\circ_{\mathrm{v}}}(T). \end{aligned}$$

This shows that

$$Q_{\mathrm{v}}(T) = p_{B^\circ_{\mathrm{v}}}(T)$$

and the totality of the family of bounded sets ensures that we obtain the strong dual topology from this family of seminorms. ■

This next proposition gives us the desired structure of observables in terms of the spectral projections.

4.10 Proposition The spectral projections for the number operator extend to surjective maps

$$P_\Xi : \mathcal{W}' \to \mathcal{H}_\Xi,$$

which we indicate by the same symbols.

For any operator $A \in \mathcal{L}(\mathcal{W}, \mathcal{W}')$ define the component operators

$$A_{\Xi\Upsilon} : \mathcal{W} \to \mathcal{H}_\Xi \subset \mathcal{W}$$

by means of these projections:

$$A_{\Xi\Upsilon} = P_\Xi A P_\Upsilon.$$

Notice that

$$A_{\Xi\Upsilon} v = \langle \Omega_\Xi, A\Omega_\Upsilon \rangle \langle \Omega_\Upsilon, v \rangle \Omega_\Xi.$$

So $A_{\Xi\Upsilon}$ can be regarded as a bounded operator from $\mathcal{H}_\Upsilon$ to $\mathcal{H}_\Xi$ with norm $|\langle \Omega_\Xi, A\Omega_\Upsilon \rangle|$.

Then the topology of uniform convergence on bounded subsets is determined by the seminorms

$$\|A\|_{\mathrm{v}} = \sum_{\Xi,\Upsilon} \|A_{\Xi\Upsilon}\| v_\Xi v_\Upsilon. \tag{4.16.a}$$

Conversely, given any matrix $(A_{\Xi\Upsilon})$ for which $\|A\|_{\mathrm{v}}$ is finite for all $\mathbf{v} \in \Gamma\left(\vec{N}, \vec{t}\right)$, the sequence $\left(A^{(\Theta)}\right)$ converges to an element $A \in \mathcal{L}(\mathcal{W}, \mathcal{W}')$, where

$$A^{(\Theta)} = \sum_{\Xi,\Upsilon \preceq \Theta} A_{\Xi\Upsilon}. \tag{4.16.b}$$

Proof The first part was shown during the proof of the previous result, when we defined the components T_Ξ. Combining the characterization of both $\mathcal{W}$ and its dual space as sequences with the technique used in the proof of Proposition [2.16] will prove the remainder of this proposition, and we refer to Lassner [4] for details. ■

We can now prove that the completion of the algebra of observables is $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$.

4.11 Proposition The algebra $\mathcal{L}^+(\mathcal{W})[\mu]$ is sequentially dense in $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$.

Proof We already know that $\mathcal{L}^+(\mathcal{W})[\mu]$ is a subspace of $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$, and that μ is the subspace topology.

The previous proposition implies that if $A \in \mathcal{L}_b(\mathcal{W}, \mathcal{W}')$, the sequence

$$A^{(\Theta)} = \sum\nolimits_{\Xi, \Upsilon \preceq \Theta} A_{\Xi\Upsilon},$$

defined in equation (4.16.b) , converges to A. This is seen from the identity

$$\left\|A - A^{(\Theta)}\right\|_{\mathrm{v}} = \sum\nolimits_{\Xi, \Upsilon \succ \Theta} \|A_{\Xi\Upsilon}\| \, v_\Xi v_\Upsilon.$$

For each Θ, the approximant $A^{(\Theta)}$ is an endomorphism of $\mathcal{W}$. Remembering that the transpose is a continuous map on $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$, the adjoint of each $A_{\Xi\Upsilon}$ is an endomorphism of $\mathcal{W}$; hence so is the adjoint of $A^{(\Theta)}$. Then every element $A \in \mathcal{L}_b(\mathcal{W}, \mathcal{W}')$ is the limit of a convergent sequence $(A^{(\Theta)})$ of elements of $\mathcal{L}^+(\mathcal{W})[\mu]$, and we are done. ■

As $\mathcal{W}$ is a nuclear Fréchet space, we know that

$$\mathcal{L}_b(\mathcal{W}, \mathcal{W}') \cong \mathcal{W}' \widehat{\bigotimes} \mathcal{W}'$$

is a tensor product, but there is no tensor product representation for the algebra of observables, so far as we know. Its dual, in contrast, is seen to have a very simple tensor product representation, in (b) below.

4.12 Corollary (a) $\mathcal{L}^+(\mathcal{W})[\mu]$ is a nuclear locally convex *–algebra .

(b) We have the isomorphism

$$\mathcal{L}^+(\mathcal{W})'_b \cong \mathcal{W} \widehat{\bigotimes} \mathcal{W}.$$

(c) $\mathcal{L}^+(\mathcal{W})$ is quasi barreled but not barreled.

Proof (a) $\mathcal{L}^+(\mathcal{W})[\mu]$ is a subspace of a nuclear space.

(b) Algebraically, the isomorphism follows from Proposition [4.11]. The topological equivalence follows because $\mathcal{L}^+(\mathcal{W})[\mu]$ is a large subspace of $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$. That is, every bounded subset of $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$ is contained in the $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$ closure of a bounded subset of $\mathcal{L}^+(\mathcal{W})[\mu]$. This is so because the approximants $A \to A^{\Theta}$ form an equicontinuous family from $\mathcal{L}_b(\mathcal{W}, \mathcal{W}')$ to itself.

(c) Were $\mathcal{L}^+(\mathcal{W})[\mu]$ barreled, the product would be hypocontinuous. The product of two bounded sets would then be bounded, which would imply that $\mathcal{L}^+(\mathcal{W})[\mu]$ was complete. We know this not to be the case, cf, Remark [4.26] below, so $\mathcal{L}^+(\mathcal{W})[\mu]$ is not barreled.

Large subspaces of quasi barreled spaces are quasi barreled, cf, Perez–Carreras and Bonet [1]. ■

4.13 Remarks (a) Much of what we have just proved depended only upon the fact that we started from a domain of the form $\mathcal{D} = \mathcal{C}^{\infty}(T)$ for some strictly positive self adjoint operator T. Lassner [4,5] has analyzed this situation in detail, including the case where $T = \int t\, E(dt)$ has a continuous spectrum. For this extension we must refer the reader to the literature.

(b) It is a consequence of the special nature of $\mathcal{W}$ that if $\mathcal{W} = \mathcal{W}_1 \widehat{\bigotimes} \mathcal{W}_2$ is composed of two species of particles, and $\mathcal{A}_j$ are the corresponding observable algebras, then

$$\mathcal{A}_1 \bigotimes \mathcal{A}_2 \subseteq \mathcal{A}$$

densely, and the μ topology inherited by the product algebra is equivalent to the projective tensor product topology, $\mu_1 \otimes_{\pi} \mu_2$. This proceeds inductively to cover the general system.

For $\mathcal{W}$ referring to one type of particle, a symmetric or antisymmetric tensor product occurs. The same result prevails. For two particles, for example, $\mathcal{W} = \mathcal{W}_1 \widehat{\bigotimes}_{\pm} \mathcal{W}_2$. Then

$$\mathcal{A}_1 \bigotimes_{\pm} \mathcal{A}_2 \subseteq \mathcal{A}$$

with the subspace topology equivalent to $\mu_1 \otimes_{\pm,\pi} \mu_2$.

This accords with the interpretation of the model physically. It states that any multiparticle observable may be approximated arbitrarily closely by single particle observables, respecting the symmetries. ■

There are other topological properties of the algebra $\mathcal{L}^+(\mathcal{W})$ that can be shown, but we must introduce the order topology to do so.

4.3 ORDER PROPERTIES

At the beginning of Chapter 3 we defined the algebraic wedge $\mathcal{P}(\mathcal{A})$ associated with any *–algebra $\mathcal{A}$. The observable algebra $\mathcal{L}^+(\mathcal{W})$ has a second wedge, in fact a cone, which is more useful for most purposes, and which we now consider. The reader will recall from Chapter 3 the decomposition

$$\mathcal{L}^+(\mathcal{W}) = \mathcal{L}^+(\mathcal{W})_h + i\,\mathcal{L}^+(\mathcal{W})_h \tag{4.17.a}$$

$$a = a_1 + ia_2, \tag{4.17.b}$$

valid for any complex vector space, here applied to the observable algebra.

It will be seen that many of the following results are valid for general op*-algebras, and so there will be no confusion if we drop the particle number and type indices, and consider a general system, with the wave function space denoted simply as $\mathcal{W}$. Here is the definition of the new positive cone.

4.14 Definition The *strong* positive cone on $\mathcal{L}^+(\mathcal{W})$ is defined to be the set

$$\mathcal{K}\left(\mathcal{L}^+(\mathcal{W})\right) = \left\{ a \in \mathcal{L}^+(\mathcal{W}) : \langle x, ax\rangle \geq 0, \quad \forall x \in \mathcal{W} \right\}. \tag{4.18.a}$$

We denote the order relation it defines by

$$a \preceq b \qquad \text{if and only if} \qquad b - a \in \mathcal{K}. \tag{4.18.b}$$

■

As $a \to \langle x, ax\rangle$ is a continuous linear functional on $\mathcal{L}^+(\mathcal{W})$ for all $x \in \mathcal{W}$, $\mathcal{K}$ is closed. The reader is advised not to confuse this strong positive order relation with either the positive order relation from $\mathcal{P}(\mathcal{A})$ or the order relation of the previous section associated with the symmetry requirements. In general,

$$\mathcal{P}(\mathcal{A}) \subset \mathcal{K}$$

for op* – algebras $\mathcal{L}^+(X)$. However, we have the following result pertinent to our model, cf, Hennings [1]. In that paper, the proposition is a corollary of various results concerning the order properties of the the dual space, $\mathcal{A}'$. For that reason, and because we do not use it in what follows, we present it without proof.

4.15 Proposition The strong positive cone $\mathcal{K}$ is the closure in $\mathcal{L}^+(\mathcal{W})[\mu]$ of the algebraic cone $\mathcal{P}(\mathcal{A})$, which follows because their topological dual wedges are equal. ■

We remark that the definition states that $\mathcal{K}$ is a proper cone, not just a wedge. This is because every element of $\mathcal{K}$ is a positive operator in the usual Hilbert space sense, hence hermitian.

Then if a is an element of both $\mathcal{K}$ and $-\mathcal{K}$,

$$\langle x, ax\rangle = 0$$

for all x. By polarization, this implies that $a = 0$. That is, $\mathcal{K}$ is proper:

$$\mathcal{K} \bigcap -\mathcal{K} = \{0\}.$$

Note that the defining condition for $\mathcal{K}$ is linear in the observables. This means that if $\mathcal{B}$ is a *-subalgebra of $\mathcal{L}^+(\mathcal{W})$, the strong positive cone on $\mathcal{B}$ coincides with the cone induced on $\mathcal{B}$ from $\mathcal{K}$.

That is,

$$\mathcal{K}(\mathcal{B}) = \mathcal{K}(\mathcal{L}^+(\mathcal{W})) \bigcap \mathcal{B}. \tag{4.19}$$

Now $\mathcal{K}$ is proper and $\mathcal{A}$ is unital, so equation (3.40) tells us that $\mathcal{K}$ is generating:

$$\mathcal{A}_h = \mathcal{K} - \mathcal{K}. \tag{4.20}$$

(Although (3.40) was stated for the algebraic cone, it evidently holds for any positive cone on a unital *–algebra which contains $\mathcal{P}$.) For a C^*–algebra, the two cones $\mathcal{K}$ and $\mathcal{P}$ coincide, and every positive element can be written in the form a^*a. This is also true for a large class of algebras called GB^*–algebras, which contains the b^*–algebras. For a proof see Allen [2] and Dixon [1]. There does not seem to be any result determining exactly which class of algebras this is true for, although special cases are known, evidently.

4.16 Notational Convention Unless otherwise specified we shall be considering only wave function spaces

$$\mathcal{W} = C^\infty(M)$$

for one of the compound systems Σ previously described. The corresponding algebra we shall consider will be $\mathcal{L}^+(\mathcal{W})$, usually with its uniform topology μ. Therefore it is not only safe to omit the $\left(\vec{N}, \vec{t}\right)$ indices, but to abbreviate the algebra of observables to

$$\mathcal{L}^+(\mathcal{W}) = \mathcal{A}$$

until further notice.

Again unless otherwise specified we shall consider only the positive cone $\mathcal{K}$ on $\mathcal{A}$. There is no reason, therefore, to refer to it as the *strong* positive cone.

Consequently there will be no ambiguity in simply referring to those subsets of $\mathcal{A}_h$ of the form

$$[\![a, b]\!] = \{ c \in \mathcal{A}_h : a \preceq c \preceq b, \ a, b \in \mathcal{A}_h \}. \tag{4.21}$$

as *order intervals*. ■

Recall from our discussion of order properties in Chapter 3, one of the most important properties that a positive cone in a *–algebra may possess is that of *normality*.

4.17 Proposition The positive cone $\mathcal{K}$ of the observable algebra $\mathcal{A}[\mu]$ is normal. Hence

(a) every order bounded subset B of $\mathcal{A}_h$ is bounded for the uniform topology.

(b) given two nets (a_i), (b_i) in $\mathcal{K}$ such that $a_i \preceq b_i$ for all i, if $b_i \to 0$, then $a_i \to 0$;

(c) if E is a real linear subspace of $\mathcal{A}_h$, then $\mathcal{K} \bigcap E$ is a normal cone in E for the subspace topology;

(d) as the uniform topology is not normable, the interior of $\mathcal{K}$ is empty.

Proof Results (a)–(d) are just a selection of the consequences of normality, and may be read off from, eg, Peressini [1] or Schaeffer [1]. Normality, recall, is defined to hold if there is a basis of seminorms such that

$$p_i(a) \ \leq \ p_i(a + b)$$

for all i and all a, $b \in \mathcal{K}$.

This condition holds for the seminorms p_{v} of equation (4.11) . To see this, let a, $b \in \mathcal{K}$. Then for every $\mathrm{v} \in \Gamma$,

$$\begin{aligned} p_{\mathrm{v}}(a + b) &= \sup \{ \langle x, ax \rangle + \langle x, bx \rangle : x \in B_{\mathrm{v}} \} \\ &\geq \sup \{ \langle x, ax \rangle : x \in B_{\mathrm{v}} \} \\ &= p_{\mathrm{v}}(a) \end{aligned}$$

and we are done. ■

For the algebra $\mathcal{A}$, the normality of $\mathcal{K}$ implies that the order topology is Hausdorff, cf, Peressini [1]. A well known general construction enables us to exhibit the seminorms for the order topology explicitly, Peressini [1], Jurzak [1], Schmüdgen [5].

4.18 Proposition Let the order topology ρ on $\mathcal{A}$ be the finest locally convex topology, Hausdorff or not, for which every order interval is ρ-bounded.

(a) For each $a \in \mathcal{K}$, define an extended real valued map on $\mathcal{A}$ by the formula

$$\rho_a(c) = \inf \{ \lambda > 0 : |\langle x, cx \rangle| \leq \lambda |\langle x, ax \rangle|, \ \forall x \in \mathcal{W} \}, \qquad (4.22.a)$$

with the convention that the infimum of the empty set is $+\infty$.

Then ρ_a is a norm on the space

$$\mathcal{N}_a = \{ c \in \mathcal{A} : \rho_a(c) < \infty \}. \qquad (4.22.b)$$

If we consider the embedding maps $\mathcal{N}_a \to \mathcal{N}_b$ for a, $b \in \mathcal{K}$ with $a \prec b$, the family $\{ \mathcal{N}_b : b \in \mathcal{K} \}$ is an inductive system.

The identification maps

$$\iota_a : \mathcal{N}_a \to \mathcal{A}$$

induce an inductive topology on $\mathcal{A}$. This is Hausdorff and equal to the order topology ρ. Consequently we may write

$$\mathcal{A}[\rho] = \lim \operatorname{ind} \{ \mathcal{N}_b, \iota_b : b \in \mathcal{K} \}, \qquad (4.22.c).$$

(b) Let us write

$$\mathcal{N}_r = \mathcal{N}_{M^r} \qquad \rho_r = \rho_{M^r} \qquad \text{and} \qquad \iota_r = \iota_{M^r}.$$

Then $\mathcal{A}[\rho]$ is the inductive limit of the family $\{ \mathcal{N}_r, \iota_r : r \geq 0 \}$,

$$\mathcal{A}[\rho] = \lim \operatorname{ind} \{ \mathcal{N}_r, \iota_r : r \geq 0 \}. \qquad (4.23)$$

Note that this countable inductive limit is not strict.

Proof Let $\mathcal{M} \subset \mathcal{N}_a$ be bounded. Then there exists a positive constant K such that

$$|\langle x, bx \rangle| \leq K \, \langle x, ax \rangle, \qquad b \in \mathcal{M}, \, x \in \mathcal{W}.$$

If $\mathcal{M} \subset \mathcal{N}_a \bigcap \mathcal{A}_h$ as well, this implies that $\mathcal{M} \subset [\![-Ka, Ka]\!]$, so $\mathcal{M} \subset \mathcal{A}[\rho]$ is bounded. Thus the embedding $\mathcal{N}_a \to \mathcal{A}[\rho]$ is locally bounded. Now $\mathcal{N}_a$ is metrizable, hence bornological, so the embedding is continuous. This is true for all $a \in \mathcal{K}$, and so the map $\mathcal{A}[\tau] \to \mathcal{A}[\rho]$ is continuous, where τ is the inductive topology defined by the embeddings. Thus $\rho \leq \tau$, implying that τ is Hausdorff; then

$$\mathcal{A}[\tau] = \lim \operatorname{ind} \{ \mathcal{N}_a, \iota_a : a \in \mathcal{K} \}.$$

Consider next an order interval $[\![a, b]\!]$ with $a,\ b \in \mathcal{A}_h$, and let $c \in \mathcal{K}$ be such that $[\![a, b]\!] \subset [\![-c, c]\!]$. Then $[\![a, b]\!] \subset \mathcal{N}_c$ and $\rho_c(d) \leq 1$ for all $d \in [\![a, b]\!]$. Thus $[\![a, b]\!]$ is bounded in $\mathcal{N}_c$, and hence bounded in $\mathcal{A}[\tau]$, showing that $\tau \leq \rho$. Then $\rho = \tau$ and equation (4.22.c) follows.

(b) For $k \in \mathcal{K}$, consider

$$\begin{aligned} |\langle x, kx\rangle| &\leq \|kx\|\ \|x\| \\ &\leq C\, \|x\|_r\ \|x\|_0 \\ &\leq C\, \|x\|_r^2, \end{aligned}$$

the last step coming from continuity. This shows that $k \leq CM^{2r}$, and we are done. ■

Equation (4.23) shows that $\mathcal{A}$ is what is sometimes termed *countably dominated*. The next step is to prove that the order topology is equivalent to the uniform topology. We begin by noticing that ρ and μ have the same bounded sets.

4.19 Lemma For a subset $\mathcal{M}$ of $\mathcal{A}$, the following three conditions are equivalent: (i) $\mathcal{M}$ is μ bounded. (ii) There is an $r \in \mathbb{N}$ and a positive constant C such that for every $m \in \mathcal{M}$ and every $x \in \mathcal{W}$,

$$|\langle x, mx\rangle| \leq C\, \|x\|_r^2.$$

(iii) $\mathcal{M}$ is ρ bounded.

Proof *(iii)* $\Rightarrow$ *(i)* is true because the cone is μ normal, so order bounded sets are μ bounded.

(ii) $\Rightarrow$ *(iii)* is true because the inequality in *(ii)* implies that $\mathcal{M}$ is a bounded subset of $\mathcal{N}_r$.

To prove *(i)* $\Rightarrow$ *(ii)*, assume that it is not true. This implies that we can find a μ bounded set $\mathcal{M}$ and a sequence $V = (x_r)$ of vectors in $\mathcal{W}$ and operators (m_r) in $\mathcal{M}$ with

$$\|x_r\|_r = 1$$

and

$$|\langle x_r, m_r x_r\rangle| \geq r.$$

Now

$$\sup\{\, \|x\|_r : x \in V\,\} \leq \max(1, \|x_0\|_r, \ldots, \|x_{r-1}\|_r), \qquad \forall r \in \mathbb{N},$$

showing that V is a bounded subset of $\mathcal{W}$. However,

$$p_{V,V}(m_r) \geq |\langle x_r, m_r x_r \rangle| \geq r, \qquad \forall r \in \mathbb{N}.$$

This implies that $\mathcal{M}$ is not μ bounded. This contradiction completes the proof of the lemma. ■

For the remainder of the proof of the equivalence of the topologies we shall suppose that $\mathcal{W}$ is just the sequence space $s^{(1)}$, for simplicity. The following approach to the equality of the μ and ρ topologies is due to Hennings [1], and holds for all nuclear Fréchet spaces possessing a basis orthonormal with respect to a given continuous inner product. This result was first shown by Schmüdgen [5], who employed a different method.

4.20 Lemma Let

$$\{\, u_n : u_n(w_m) = \delta_{nm} \,\}$$

be the family of coordinate functionals dual to the Schauder basis $\{\, w_n : n \geq 0 \,\}$ of $s^{(1)}$. These functionals constitute a Schauder basis for $\left[s^{(1)}\right]_b'$. The family $\{\, u_{nm} : n, m \geq 0 \,\}$, where

$$u_{nm} = u_n \otimes u_m, \tag{4.24}$$

constitutes a Schauder basis for $\left[s^{(1)}\right]_b' \widehat{\otimes} \left[s^{(1)}\right]_b'$. The linear span of this basis, call it $\mathcal{F}$, is sequentially dense. ■

With these notational conventions, the elements u_{nm} are scalar multiples of the operators $A_{\Xi\Upsilon} \in \mathcal{A}$ mentioned in Proposition [4.10]. This allows us to identify $s^{(1)\prime} \widehat{\otimes} s^{(1)\prime}$ with a subspace of $\mathcal{A}$, and hence $\mathcal{F}$ with a subspace of $\mathcal{A}$.

For brevity we shall now write

$$s_2^{(1)} = s^{(1)} \widehat{\bigotimes} s^{(1)}, \tag{4.25.a}$$

$$[s_2^{(1)}]_b' = [s^{(1)}]_b' \widehat{\bigotimes} [s^{(1)}]_b'. \tag{4.25.b}$$

We want to show that $\mathcal{F}$ is bornological. For this purpose, it is convenient to have a certain representation of $[s_2^{(1)}]_b'$ available.

4.21 Lemma Let $\mathcal{H}_{rr}$ be the completion of $s_2^{(1)}$ in the metric topology defined by the inner product

$$\langle x_1 \otimes y_1 \,, x_2 \otimes y_2 \,\rangle_{rr} = \langle x_1 \,, x_2 \,\rangle_r \, \langle y_1 \,, y_2 \,\rangle_r .$$

We have employed our usual notation for the inner products associated with the powers of the number operator.

Then $s_2^{(1)}$ is the reduced projective limit of the $\mathcal{H}_{rr}$. By duality and the reflexivity of $s_2^{(1)}$, it follows that $[s_2^{(1)}]_b'$ is the countable inductive limit of the $\mathcal{H}_{rr}$, which are self dual. ■

This is a simple rereading of previous work and so we omit the proof. We remind the reader that the projective tensor product topology may be obtained through the indicated inner products.

4.22 Lemma The subspace $\mathcal{F}$ is bornological

Proof Write $\mathcal{F}_{rr}$ for $\mathcal{F}$ with the $\mathcal{H}_{rr}$ metric topology. Let Y be any B- space and f a linear map from $\mathcal{F}$ into Y which is bounded on bounded subsets. As metrisable spaces are bornological, f is continuous on $\mathcal{F}_{rr}$. Therefore it extends continuously to $\mathcal{H}_{rr}$. We write f_{rr} for the extension.

It is possible to define a map $g : [s_2^{(1)}]_b' \to Y$ whose restriction to $\mathcal{H}_{rr}$ is f_{rr} for all r. We omit the proof, and refer the reader to Hennings [1] for details.

As $[s_2^{(1)}]_b'$ is an inductive limit, the continuity of all the f_{rr} implies that g is continuous, and so f, the restriction of g to $\mathcal{F}$, is continuous. As Y was arbitrary, $\mathcal{F}$ is bornological. ■

Even though $\mathcal{A}[\mu]$ is sandwiched sequentially densely between two bornological spaces, we cannot conclude from this alone that it is itself bornological. There is, however, a form of sequential density which is designed for just such a purpose.

4.23 Proposition A sequence (x_n) in an *lcs* E converges locally to x if there exists a sequence (c_n) of positive numbers diverging to $c_n \to \infty$, and such that

$$c_n(x_n - x) \to 0.$$

The sequence $(x_n - x)$ is then said to be a locally null sequence.

An *lcs* is bornological if and only if every absolutely convex subset which absorbs all locally null sequences is a neighbourhood of zero.

A subspace F of an *lcs* E is locally dense if every element x of E is the limit of a locally convergent sequence from F. If this is the case and F is bornological, then so is E, cf, Perez–Carreras and Bonet [1]. ■

It is this last condition which is useful here. All we need to do is prove that $\mathcal{F}$ is locally dense in $\mathcal{A}[\mu]$.

4.24 Proposition $\mathcal{F}$ is locally dense in $\mathcal{A}[\mu]$. Hence μ is bornological and so equal to ρ. Hence μ is the finest locally convex topology such that the positive cone is normal.

Proof We start with the observation that if $T \in [s^{(1)}]'$, then so is

$$S_n = (n+1)^r \, T_n$$

for any fixed r. This result holds for $[s_2^{(1)}]'_b$, with

$$S_{nm} = (n+1)^r (m+1)^s \, T_{nm}$$

for fixed r and s.

Let $T \in [s_2^{(1)}]'_b$ be arbitrary, and write

$$T^{(N)} = \sum_{n,m \leq N} T_{nm} u_{nm}$$

for the N-th approximant to T as in the proof of sequential density Proposition [4.11].

If we scale in $(n+1)$ to T as above, with r and s equal to 1, we get an element S. Similarly for the approximant $S^{(N)}$ to it.

Let

$$R^{(N)} = S - S^{(N)}$$

be the remainder. From sequential density we know that

$$\lim_{N \to \infty} \left\| R^{(N)} \right\|_r = 0, \qquad \forall r.$$

This implies the local convergence of $T^{(N)}$ to T, with the choice of the sequence

$$c_n = (n+1)^2,$$

so μ is bornological. Since both ρ and μ are bornological and have the same bounded sets, the identity map from $\mathcal{A}[\mu]$ to $\mathcal{A}[\rho]$ is a topological isomorphism, so $\mu = \rho$.

Using the same technique as in Lemma [4.19], we deduce that $\mu = \rho$ is finer than any locally convex topology for which the cone is normal, and the proof is complete.

■

Now that we have shown that the order topology is equivalent to the uniform topology it must follow that positivity is related to continuity. In what follows we shall assume that $\mathcal{A}$ is equipped with its μ topology unless the contrary is noted.

Recall that a set is order bounded if it is a subset of an order interval. A map between ordered vector spaces is positive if it maps the positive cone into the positive cone, and is order bounded if it maps order bounded sets into order bounded sets. Positive maps are order bounded.

4.25 Corollary (a) A positive map from $\mathcal{A}$ to itself is necessarily continuous.

(b) All positive linear functionals on $\mathcal{A}$ are necessarily continuous.

(c) The set of all order bounded linear functionals on $\mathcal{A}$ coincides with set of all continuous linear functionals, $\mathcal{A}'$.

Proof (a) and (b) are consequences of the facts that μ is bornological and $\mathcal{K}$ is normal; and (c) is trivial. ■

4.26 Remarks It is not true that for an arbitrary bounded subset $\mathcal{B}$ of $\mathcal{A}$ its square

$$\mathcal{B}^2 = \{\, ab : a, b \in \mathcal{B} \,\} \tag{4.26}$$

is bounded, as this would imply the completeness of $\mathcal{L}^+(\mathcal{W})[\mu]$. This is only possible for nuclear Fréchet $\mathcal{W}$ when $\mathcal{W}$ is finite dimensional.

$\mathcal{A}$ is neither semi reflexive nor barreled, but it is quasi barreled. We remind the reader that as a subspace of a nuclear space, its completion, it is nuclear.

The sequential density of the span $\mathcal{F}$ of the basis elements of $[s_2^{(1)}]_b'$ can be stated as asserting that the finite rank operators in $\mathcal{A}$ are dense. The usual terminology for this is that $\mathcal{A}$ has the finite approximation property. In fact we know it has the stronger property of local density. This is also clearly the case for general $\mathcal{W}$. ■

4.4 COMPLETE SETS OF COMMUTING OBSERVABLES

In this section we discuss complete sets of commuting observables, a notion introduced by Dirac. As defined in his book, the idea seems to be that the space of wave functions should be a Fréchet space with a Schauder basis. It would seem that for physical reasons such a basis will be indexed by elements of a subset of $\mathbb{N}^d$, call it Λ. Then

$$L_j\, e(\lambda_1, \ldots, \lambda_d) \;=\; \lambda_j\, e(\lambda_1, \ldots, \lambda_d)$$

serves to define operators L_j with simple discrete spectra and the basis vectors as eigenvectors. The L_j mutually commute on the linear span of the basis vectors, and Dirac terms the family $(L_j \,:\, 1 \leq j \leq d)$ a complete set of commuting observables, or CSCO for short.

He also supposes that given a finite set of observables, one can choose a maximally independent subset from them. Supplementing them by further observables if needs be, a CSCO is determined. In this way, a quantum mechanical system can be described by a largest set of commuting and diagonalized observables, chosen for maximum convenience.

In our formulation it is certainly the case that the space $\mathcal{W}$ of wave functions is Fréchet , and even that

$$\mathcal{W} = \mathcal{C}^{\infty}(\mathrm{M}).$$

We could then say that the Cartesian component number operators $(M_j : 1 \leq j \leq d)$ form a CSCO.

Several variants of these ideas have been analyzed in the literature. Perhaps the best known is that of a maximal abelian von Neumann algebra. This is a von Neumann algebra which coincides with its commutant. In terms of Dirac's original idea, this sort of algebra arises as the bicommutant of the spectral projections along the basis elements.

The question arises as to whether it is possible to introduce a generalized commutant for, say, an op* − algebra. This would have to reduce to a maximal abelian von Neumann algebra in the bounded case. It would also have to allow of the number operators above as an example.

As we are dealing with unbounded operators, an immediate complication arises. There are examples known of unbounded operators which commute on a domain of essential self adjointness, but whose spectral projections do not commute.

The following example is due to Nelson, and is given in Reed and Simon [1]. Let $\mathcal{M}$ be the Riemann surface for $\sqrt{z}$, and consider the Hilbert space $L^2(\mathcal{M})$ with local Lebesgue measure. We define

$$a = -i\partial/\partial x \quad \text{and} \quad b = -i\partial/\partial y$$

on the domain of $\mathcal{C}^{\infty}$ functions of compact support excluding the origin.

This cannot happen for bounded operators of course. Hereafter, then, when we say that two operators commute, we mean that their spectral projections commute.

The following three types of commutants appear on this context, but the reader will discern that yet others can be defined. We take this opportunity to introduce formally the notion of an *op**–algebra , due to Lassner [1-6].

4.27 Definition Let D be a Fréchet space, equipped with a continuous inner product. The completion of D with respect to this inner product is a Hilbert space, denoted $\mathcal{H}$.

By $C(D, \mathcal{H})$ we mean the set of all closable operators from D into $\mathcal{H}$. As both of these spaces are Fréchet , such operators are continuous by the closed graph theorem. But note that such an operator is not continuous when D has its subspace topology inherited from $\mathcal{H}$ unless it is bounded.

By an op* – algebra we mean a unital subalgebra of $\mathcal{L}^+(D)$. The conditions may be relaxed to include domains which are neither metrizable nor complete, but they must be pre-Hilbert spaces.

Let $\mathcal{B}$ be an op* – algebra on the domain D. The unbounded weak commutant of $\mathcal{B}$ is

$$\pi(\mathcal{B})'_\sigma = \left\{ a \in C(D, \mathcal{H}) : \langle ax, by\rangle = \langle ab^+ x, y\rangle, \quad x, y \in D,\ b \in \mathcal{B} \right\}. \tag{4.27.a}$$

We write

$$\pi(\mathcal{B})''_{\sigma\sigma} = \left(\pi(\mathcal{B})'_\sigma\right)'_\sigma. \tag{4.27.b}$$

The bounded weak commutant is

$$\pi(\mathcal{B})'_w = \left\{ a \in \mathcal{L}(\mathcal{H}) : \langle ax, by\rangle = \langle b^+ x, a^* y\rangle, \quad x, y \in D,\ b \in \mathcal{B} \right\}, \tag{4.27.c}$$

and the bounded strong commutant is

$$\pi(\mathcal{B})'_s = \{ a \in \mathcal{L}(\mathcal{H}) : a D \subseteq D,\ bax = abx,\ x \in D,\ b \in \mathcal{B} \}. \tag{4.27.d}$$

■

We present, without proof, a selection of results concerning these sets.

4.28 Proposition (a) The weak commutant $\pi(\mathcal{B})'_w$ is a linear subspace of $\mathcal{L}(\mathcal{H})$, closed in the weak operator topology. It contains the unit operator and is *-symmetric. It is the linear span of its positive elements, but is not an algebra in general.

(b) $\pi(\mathcal{B})'_s$ is an algebra contained in $\pi(\mathcal{B})'_w$. If $\mathcal{B}$ is self adjoint, then the weak and strong bounded commutants coincide.

(c) $\pi(\mathcal{B})'_\sigma$ and $\pi(\mathcal{B})''_{\sigma\sigma}$ are *-symmetric linear subspaces of $C(D, \mathcal{H})$, and are closed in the relative $\mathcal{L}_s\left(D, \mathcal{H}\left[\sigma(\mathcal{H}, \mathcal{H}')\right]\right)$ topology. $\pi(\mathcal{B})'_w$ is the bounded part of $\pi(\mathcal{B})'_\sigma$:

$$\pi(\mathcal{B})'_w = \pi(\mathcal{B})'_\sigma \bigcap \mathcal{L}(\mathcal{H}).$$

If $\mathcal{B}$ is self adjoint $\pi(\mathcal{B})'_\sigma$ is a subset of $\mathcal{L}^+(D)$. ■

We now have enough material to define a CSCO in the maximal op* – algebra setting. The definition we give may be extended to non maximal op* – algebras.

4.29 Definition A complete set of commuting observables for $\mathcal{L}^+(D)$ is a finite set of hermitian operators

$$\mathcal{Q} = \{\, a_1, \ldots, a_n : a_j \in \mathcal{L}^+(D)_h \,\}$$

for which

$$(i) \qquad \mathcal{C}^\infty(a_1, \ldots, a_n) = D$$

$$(ii) \qquad \pi\left(\mathcal{L}^+(D)\right)'_w = \pi\left(\mathcal{L}^+(D)\right)'_s$$

$$(iii) \qquad \pi\left(\mathcal{L}^+(D)\right)'_w = \pi\left(\mathcal{L}^+(D)\right)''_{ww}.$$

■

The principal result of this definition is as follows.

4.30 Proposition Let $\mathcal{Q}$ be a complete set of commuting observables for $\mathcal{L}^+(D)$. Then D contains a dense set of vectors which are analytic for all the a_j. D is stable under, and a core for, each a_j.

The operator

$$T = \left[\sum_{j=1}^{n} a_j^2 | D\right]^{**}$$

is self adjoint and determines the domain:

$$D = \mathcal{C}^\infty(T).$$

Under these circumstances, the bounded weak commutant is a W^*–algebra .

$\mathcal{Q}$ is a CSCO for $\mathcal{L}^+(D)$ if and only if

$$\pi(\mathcal{P}(\mathcal{Q}))'_\sigma = \pi(\mathcal{P}(\mathcal{Q}))''_{\sigma\sigma},$$

where $\mathcal{P}(\mathcal{Q})$ is the poynomial op* – algebra generated by $\mathcal{Q}$.

$\mathcal{Q}$ is a CSCO for $\mathcal{L}^+(D)$ if and only if there exists a normalized vector $\Omega \in D$ which is cyclic in the sense that $\pi(\mathcal{P}(\mathcal{Q}))''_{\sigma\sigma}\Omega$ is dense in $\mathcal{H}$. ■

For a proof we refer the reader to Antoine, Epifanio and Trapani [1], and Epifanio and Trapani [1]. We present the following examples also without proofs, which can be found in the above references.

4.31 Examples (i) For the space of wave functions $\mathcal{W}$ which we have been considering, the number operator components constitute a CSCO for the algebra of observables $\mathcal{A}$, as required.

(ii) For one degree of freedom, recall that the kinetic energy operator is proportional to the square of the number operator minus a constant. A CSCO for one degree of freedom is the kinetic energy operator, the square of the angular momentum, and one of its components,

$$\mathcal{Q} = \{T, \mathbf{L}\cdot\mathbf{L}, L_z\}.$$

This generalizes to d degrees of freedom in an obvious way.

(iii) The set of all coordinates is not a CSCO for $\mathcal{A}$, but it is for the algebra $\mathcal{L}^+(D)$ with D equal to the set of all elements in $L^2(\mathbb{R}^d)$ of rapid decrease at infinity.

For the set of all momenta, we get a CSCO for $\mathcal{L}^+(D)$ with D equal to the Sobolev space $H^{2,\infty}$. We remark that the bi-σ commutant contains a large class of functions of the operators in $\mathcal{Q}$. For the momenta, for example, it contains many pseudo differential operators. In particular, it contains all real powers of the Laplacian. ∎

This completes our study of complete sets of commuting observables.

4.6 IDEALS OF $\mathcal{L}^+(D)$.

In this section we wish to note, without proof, the results of an investigation by Kürsten of the family of all two sided ideals which are closed in the usual μ topology. His work concerned the case where D is a Fréchet space in the graph topology. We shall only consider two sided ideals, so shall refer simply to ideals. Similarly, we shall mean μ closed when we say closed.

A central role is played by the following sets.

4.32 Definition (a) We write

$$\mathrm{T} = \left\{ a \in \mathcal{L}^+(D) \bigcap \mathcal{L}(\mathcal{H}) : \overline{a}, \overline{a^*} : \mathcal{H} \to D \right\}, \tag{4.28.a}$$

$$\mathrm{T}_h = \left\{ a \in \mathrm{T} : a^+ = a \right\}, \tag{4.28.b}$$

$$\mathrm{P} = \left\{ a \in \mathrm{T}_h : a^2 = a \right\}. \tag{4.28.c}$$

(b) Let α, β, ... be ordinals, and $\aleph_\alpha$, $\aleph_\beta$, ... be cardinals, in a usual notation.

By $d(a)$ we mean the dimension of the Hilbert space which is the Hilbert completion of $a\,D$ for $a \in \mathrm{P}$. Define the ordinal ξ, which depends on D, by

$$\aleph_\xi = \sup\{ d(a) : a \in \mathrm{P} \},$$

where the supremum is taken in the family of cardinals.

For an ordinal $\alpha \leq \xi$, let I_α be the closed ideal generated by the observables

$$\{ a \in \mathrm{P} : d(a) < \aleph_\alpha \}.$$

■

Kürsten's principal results are contained in this next propostion.

4.33 Proposition (a) The set of all non trivial closed ideals of $\mathcal{L}^+(D)$ is given by

$$\{ \mathrm{I}_\alpha : \alpha < \xi \}.$$

If

$$\alpha < \beta < \xi,$$

then I_α is strictly contained in I_β.

(b) $\mathcal{L}^+(D)$ has at least two non trivial closed ideals if and only if D contains a non separable bounded subset.

(c) If D is a Hilbert space of dimension $\aleph_\beta$, then $\xi = \beta + 1$ and $\mathcal{L}^+(D)$ has the maximal closed ideal I_β. For D not a Hilbert space there is no maximal closed ideal, in general. In fact, one may construct a Fréchet D for which ξ is the first infinite ordinal.

(d) $\mathcal{L}^+(D)$ has at most one non trivial closed ideal if and only if $\xi \leq 1$. If there is one and only one such ideal I_0, then an observable is an element of it if and only if it maps every weakly convergent sequence of D into a convergent sequence. Such an observable may be termed completely continuous.

This situation occurs if and only if (*i*): D is not a Montel space, and (*ii*): each bounded subset of D is separable.

(e) $\mathcal{L}^+(D)$ contains no closed ideals if and only if D is a Fréchet Montel space.

■

4.34 Corollary The physical algebra of observables, $\mathcal{A} = \mathcal{L}^+(W)$, contains no closed two sided ideals. ■

This completes our initial study of the algebra of observables, $\mathcal{L}^+(W)$.

5. THE STATES OF THE SYSTEM

5.1 STATES AS POSITIVE FUNCTIONALS

Recall the definition of an observer-state system which we gave in Definition (2.1). Modified to take into account the subsequent material we now raise it to the status of an axiom, in the following form.

Axiom 4.a The set of states S for the quantum system $\Sigma_{(\vec{N},\vec{t})}$ is the set of $\mathcal{K}$-positive linear functionals on $\mathcal{A}$, normalized by $T(I) = 1$. The topology on S is that inherited as a subset of $\mathcal{A}'_b$. ∎

Recall that positivity implies continuity here. The second part of this axiom will consist of our identifying S in a concrete manner.

First, though, let us consider the background to this axiom. As we have noted before, the first idea concerning quantum states was that a state was a wave function in the Schrödinger sense. Such states were analyzed by physicists on an individual basis, so to speak. Of particular interest were states corresponding to definite energy values, and their time evolutes. Next in importance were linear combinations of such states.

This led to considering all vectors in the system Hilbert space as states. We have seen the trouble with such optimism, how it conflicts with the unbounded nature of the basic observables, and the requirement that there be a well defined mean value for every observable in a given state.

We might mention here that physicists sometimes employ the term wave function to indicate a vector in $L^2(\mathbb{R}^3)$ which is of compact support. The support of the vector is taken to be the region where the particle is. This is certainly true in the probabilistic sense. The absolute significance of the compact support property seems remote, however, since it is destroyed by the free time evolution.

Given a wave function $u \in \mathcal{W}$, information is extracted by means of matrix elements $\langle u, a u\rangle$ for observables a. As the Schrödinger representation is algebraically irreducible (Proposition [5.4] below), knowing all these matrix elements defines u up to a phase factor (Examples [3.34.5]). With Axiom 4.a defining what is meant by a state, we see that each normalized vector in $\mathcal{W}$ defines a state, up to a phase factor, by

$$T(a) = \langle u, au\rangle. \tag{5.1}$$

This is the simplest sort of linear functional on the algebra of observables.

Suppose now that the system under consideration is a subset of some larger, closed system. Using terminology from thermodynamics for convenience, the larger system will be termed the universe, and the complement of the system in the universe we shall call the reservoir. We may suppose, then, that the space of wave functions for the universe is a tensor product of the wave function spaces for the system and the reservoir.

As the universe is closed, we may suppose it to be in some state described by a wave function, say Ψ. Given an observable a for the system alone, its expected value is

$$T(a) = \langle \Psi,\, a \otimes I\, \Psi \rangle. \tag{5.2}$$

Following the general principles, we must conclude that objects such as T are necessary in order to describe non closed systems.

Examination of equation (5.2) shows that T is a positive linear functional on the algebra of the system. Unlike the wave functions we have previously encountered, however, we note that T will not be determined by a vector in the system wave function space unless the state of the universe was a product,

$$\Psi = u \otimes \xi. \tag{5.3}$$

On mathematical and physical grounds we distinguish this latter case by referring to it as a pure state. Other states are said to be mixed.

Pure states require a rather special physical circumstance in the universe. Moreover, given such a state, its purity will persist in time if and only if the system and the reservoir do not interact energetically.

Mathematically, the pure states are a subset of the extreme points of the convex set of all states. For elementary quantum systems we shall show that the pure states constitute all extreme points. In quantum field theory this is not the case, and there are pathological pure states which are not vectors.

If T is not a vector state in the system Hilbert space, what can be said about its form? Formal considerations indicate that it has the form of a trace,

$$T(a) = \operatorname{tr}(\overline{\rho a}), \tag{5.4}$$

where ρ is a positive trace class operator such that the closure of ρa is trace class for all observables a.

To see how this comes about, suppose the universe wave function is of the form

$$\Psi = \sum_{j,k=1}^{\infty} c_{jk}\, u_j \otimes \xi_k, \tag{5.5.a}$$

where the u_j and the ξ_k are orthonormal bases in the system and reservoir, respectively. The normalization of Ψ requires that

$$\sum |c_{jk}|^2 = 1. \tag{5.5.b}$$

If we combine equations (5.2) and (5.5.a), we find that

$$T(a) = \sum_{i,j,k=1}^{\infty} \overline{c_{ik}} c_{jk} T_{ij}(a), \tag{5.6.a}$$

where each

$$T_{ij}(a) = \langle u_i, a u_j\rangle \tag{5.6.b}$$

is a functional on the system.

The interpretation of this result is that we have replaced the interaction between the system and the reservoir by a statistical admixture of system functionals. If we confine our considerations to the system alone, we can determine the functionals T_{ij} and the statistical coefficients $\sum_{k=1}^{\infty} \overline{c_{ik}} c_{jk}$ by experiment. It is very important to note that this does not determine the coefficients c_{jk} completely. To know these would imply that we had a perfect knowledge of Ψ, a contradiction.

This is reminiscent of the reasoning employed in statistical mechanics, where an incomplete knowledge of the environment requires the use of systems states which are convex combinations of extremal states. These latter are said to be pure, the former being known as mixed, or impure.

One measure of the ignorance of Ψ resulting from considering the system alone is the loss of correlations between the system and the reservoir. A simple calculation shows that, in general,

$$\langle \Psi, a \otimes b\, \Psi\rangle \neq T(a)\, \langle \Psi, I \otimes b\, \Psi\rangle.$$

If we define the continuous linear map ρ by the formula

$$\rho(x) = \sum_{i,j,k=1}^{\infty} \overline{c_{ik}} c_{jk} \langle u_i, x\rangle u_j, \tag{5.7.a}$$

then ρ is a positive continuous operator on the system Hilbert space, whose trace is unity:

$$\rho \geq 0 \qquad \text{and} \qquad \operatorname{tr} \rho = 1. \tag{5.7.b}$$

Moreover, the sum in equation (5.6.a) can be written as the trace in equation (5.4). Thus, physical and statistical considerations lead us to tracial states for non closed systems.

The mathematics and the physics are then most closely matched in an algebraic model in which the set of tracial functionals exhausted the set of continuous linear functionals on the algebra. For the model where $\mathcal{A}$ is the set of all bounded operators on the system Hilbert space, there are non tracial functionals. In order to eliminate them, it is necessary to impose the further condition of σ-weak continuity. Such states are said to be normal.

In contrast we have the interesting result that no such additional requirement is necessary for the model based on $\mathcal{L}^+(\mathcal{W})$. The proof of this is our next concern.

There are a number of ways to proceed. In the next section we follow a method due essentially to Lassner and Timmermann [1]. Other treatments may be found in Sherman [1], Woronowicz [1], Schmüdgen [3,4], Hennings [1].

5.2 STATES AS DENSITY MATRICES

In Chapter 4 we have shown that $\mathcal{A}$ was a large and sequentially dense subspace of $\mathcal{W}'\widehat{\otimes}\mathcal{W}'$, cf, Proposition [4.11] and Corollary [4.12]. We know that it follows that the strong dual of $\mathcal{A} = \mathcal{L}^+(\mathcal{W})$ may be identified with the completed tensor product $\mathcal{W}\widehat{\otimes}\mathcal{W}$, which is a nuclear Fréchet space. States are those elements of $\mathcal{W}\widehat{\otimes}\mathcal{W}$ which are positive on $\mathcal{K}$ and normalized by $T(\mathbf{1}) = 1$. In this section we seek to identify the set of states with a certain class of density matrices. Note that we shall not introduce any notational distinction between an element $T \in \mathcal{A}'$ and $T \in \mathcal{W}\widehat{\otimes}\mathcal{W}$.

In the remainder of this section we shall assume that $\mathcal{W} = \mathcal{S}$ in all calculations. This merely serves to simplify the notation, and the reader should have no real difficulty in going over to the full case considered in Chapters 2 and 4.

It will turn out that $\mathcal{W}\widehat{\otimes}\mathcal{W}$ coincides with the set T introduced in Definition (4.34), in connection with ideals. We start by obtaining a new definition of T.

As usual, we write $\mathcal{W}_r$ for the Hilbert space completion of $\mathcal{W}$ in the norm $\|\cdot\|_r$. It is useful to introduce the M-norms $\|\cdot\|_r$ for negative integers r, an allowable procedure as M^{-1} is bounded, even Hilbert–Schmidt. Then

$$\mathcal{W} = \bigcap_{r\in\mathbb{Z}} \mathcal{W}_r. \tag{5.8}$$

With this, we can apply an interpolation theorem to prove the following.

5.1 Lemma (a) For any $A \in \mathcal{L}^+(\mathcal{W})$ there is an index $r \geq 0$ such that $M^{-2r}A$ and AM^{-2r} are bounded operators on $\mathcal{H}$.

(b) We may identify $\mathtt{T}$ with the following sets

$$\begin{aligned}
\mathtt{T} = \mathtt{R} &= \left\{ R \in \mathcal{L}^+(\mathcal{W}) : \overline{ARB} \text{ is trace class, } \forall A, B \in \mathcal{L}^+(\mathcal{W}) \right\}. && (5.9.a)\\
= \mathtt{R}_0 &= \left\{ R \in \mathcal{L}^+(\mathcal{W}) : \overline{M^r R M^r} \text{ is bounded, } \forall r \geq 0 \right\}. && (5.9.b)\\
= \mathtt{R}_1 &= \left\{ R \in \mathcal{L}^+(\mathcal{W}) : \overline{M^r R M^r} \text{ is trace class, } \forall r \geq 0 \right\}. && (5.9.c)\\
= \mathtt{R}_2 &= \left\{ R \in \mathcal{L}^+(\mathcal{W}) : \overline{M^r R M^r} \text{ is Hilbert–Schmidt, } \forall r \geq 0 \right\}. && (5.9.d)
\end{aligned}$$

(c) The families $\left\{ R \to \|R\|_{j,r}{}' : r \geq 0 \right\}$ are equivalent families of seminorms on $\mathtt{T}$ which define a metrisable locally convex topology, denoted α, where

$$\|R\|_{j,r}{}' = \|M^r R M^r\|_j, \qquad R \in \mathtt{T}, \ j = 0, 1, 2. \tag{5.10}$$

By $\|\cdot\|_j$ we mean the operator, trace, and Hilbert–Schmidt norm, as $j = 0, 1, 2$, respectively.

Proof Part (a) The existence of an $r \geq 0$ such that $M^{-2r}A$ is bounded is just a consequence of the fact that $A \in \mathcal{L}(\mathcal{W}[\nu])$. Since

$$AM^{-2r} \subseteq \left(M^{-2r}A^+\right)^*,$$

the existence of an $s \geq 0$ such that AM^{-2s} is bounded now follows. Obviously $M^{-2t}A$ and AM^{-2t} are bounded for all $t \geq r, s$.

(b) Clearly

$$\mathtt{R} \subseteq \mathtt{R}_1 \subseteq \mathtt{R}_2 \subseteq \mathtt{R}_0.$$

If $R \in \mathtt{R}_0$ and A, $B \in \mathcal{L}^+(\mathcal{W})$, we can find an $r \geq 0$ such that AM^{-r} and $M^{-r}B$ are bounded. Then

$$ARB = \left(AM^{-r}\right)\left(M^{-2}\right)\left(M^{r+2}RM^{r+2}\right)\left(M^{-2}\right)\left(M^{-r}B\right)$$

is a product of bounded and trace class operators, and so is itself trace class. Then

$$\mathtt{R} = \mathtt{R}_1 = \mathtt{R}_2 = \mathtt{R}_0.$$

To show that $\mathtt{T} \subseteq \mathtt{R}$ it is sufficient to to show this for symmetric elements $R = R^+$ of $\mathtt{T}$. By the closed graph theorem, we have $R \in \mathcal{L}(\mathcal{H}, \mathcal{W})$. Thus, taking the hermiticity of R and M into account, for all $s \geq 0$,

$$R \in \mathcal{L}(\mathcal{W}_{-4s}, \mathcal{H}) \bigcap \mathcal{L}(\mathcal{H}, \mathcal{W}_{4s})$$

By an interpolation theorem of Krein and Petunin [1], $R \in \mathcal{L}(\mathcal{W}_{-2s}, \mathcal{W}_{+2s})$ for all $s \geq 0$. This is equivalent to the boundedness of $M^s R M^s$, and so $R \in \mathrm{R}_0$. As we have shown that $\mathrm{R}_0 = \mathrm{R}$, we have $\mathrm{T} \subseteq \mathrm{R}$.

Conversely, if $R \in \mathrm{R}$, then $R^+ M^r R$ is bounded for all $r \geq 0$. Then

$$\|Rx\|_r^2 = \langle x, R^+ M^r R x\rangle \leq \left\|R^+ M^r R\right\| \|x\|^2$$

for all $x \in \mathcal{H}$, so that $\overline{R} \in \mathcal{L}(\mathcal{H}, \mathcal{W}_r)$ for all $r \geq 0$; hence $\overline{R} \in \mathcal{L}(\mathcal{H}, \mathcal{W})$. Clearly $\overline{R^+} \in \mathcal{L}(\mathcal{H}, \mathcal{W})$ also, so $R \in \mathrm{T}$.

(c) This follows from

$$\|R\|_{0,r}{}' \leq \|R\|_{2,r}{}' \leq \|R\|_{1,r}{}'$$

and

$$\begin{aligned}\|R\|_{1,r}{}' &= \|M^r R M^r\|_1 \\ &\leq \left\|M^{-2}\right\|_1^2 \|R\|_{0,r+2}{}'\end{aligned}$$

for all $R \in \mathrm{T}$ and $r \geq 0$, proving the proposition. ∎

The set w_j of Hermite vectors forms an orthonormal basis for $\mathcal{H}$ consisting of eigenvectors of M. This enables us to define a map $J : \mathcal{H} \to \mathcal{H}$ by setting

$$J\left(\sum\nolimits_n a_n w_n\right) = \sum\nolimits_n \overline{a_n} w_n, \tag{5.11}$$

showing that J is antilinear, with $J^2 = I$ and

$$\langle J\xi, \eta\rangle = \langle J\eta, \xi\rangle, \qquad \xi, \eta \in \mathcal{H}. \tag{5.12}$$

It is also clear that $\mathcal{W}$ is stable under J, and that, for all $r \geq 0$, M^r commutes with $J|_{\mathcal{W}}$.

We can now be more careful about the nature of the embedding of $\mathcal{H}$ into $\mathcal{W}'$ afforded by the rigged triple $(\mathcal{W}, \mathcal{H}, \mathcal{W}')$, so as to make precise the kernel nature of observables and states. The embedding in question is the map $j : \mathcal{H} \to \mathcal{W}'$ given by

$$[j\xi, x] = \langle J\xi, x\rangle \qquad \xi \in \mathcal{H}, x \in \mathcal{W}. \tag{5.13}$$

Here and until further notice, the square brackets indicate the usual bilinear duality pairing between a locally convex space and its dual; that is, without complex conjugation. The spaces in questions are to be inferred from the context.

We note that the antilinear map $k : \mathcal{W} \to \mathcal{W}'$ of equation (4.3) can be factored as

$$k = j \circ J. \tag{5.14}$$

Since $\mathcal{W} \subset \mathcal{H}$, we obtain the exact nature of the topological embedding of

$$\mathcal{L}^+(\mathcal{W})[\mu] \hookrightarrow \mathcal{L}_b(\mathcal{W}, \mathcal{W}'),$$

in that $A \in \mathcal{L}^+(\mathcal{W})$ corresponds to $j \circ A \in \mathcal{L}(\mathcal{W}, \mathcal{W}')$.

It is a standard result that the duality of $\mathcal{W} \bigotimes \mathcal{W}$ and $\mathcal{L}(\mathcal{W}, \mathcal{W}')$ is implemented by the formula

$$[x \otimes y, T] = [Ty, x], \qquad x, y \in \mathcal{W},\, T \in \mathcal{L}(\mathcal{W}, \mathcal{W}'), \tag{5.15}$$

and this then tells us that the duality of $\mathcal{W} \widehat{\bigotimes} \mathcal{W}$ and $\mathcal{L}^+(\mathcal{W})$ is implemented by the formula

$$[x \otimes y, A] = \langle Jx, Ay \rangle, \qquad x, y \in \mathcal{W},\, A \in \mathcal{L}^+(\mathcal{W}). \tag{5.16}$$

It is also elementary that J defines a continuous involution, denoted *, on $\mathcal{W} \widehat{\bigotimes} \mathcal{W}$ such that

$$(x \otimes y)^* = Jy \otimes Jx, \qquad x, y \in \mathcal{W}. \tag{5.17}$$

What we have just done is to be explicit about the fact that the duality pairing for a complex locally convex space E and its dual E' is bilinear. When E is also a pre–Hilbert space, the inner product, in contrast, is sesquilinear. Then in rigged triple cases, this distinction is maintained through a complex structure. In our case this is the operator J. The complex structure then extends the distinction to the embedding of $\mathcal{H}$ into E'.

This phenomenon has been observed by Dirac. He distinguishes bras and kets by just such an antilinear isomorphism. We shall return to bras and kets below. We now continue with our analysis of the relation between $\mathcal{A}'$ and T.

The topology $\nu \widehat{\otimes} \nu$ on $\mathcal{W} \widehat{\bigotimes} \mathcal{W}$ can be defined by the family of norms given by

$$\|T\|_r{}'' = \langle T, M^{2r} \otimes M^{2r} T \rangle^{1/2}, \qquad \text{for all } T \in \mathcal{W} \widehat{\bigotimes} \mathcal{W},\ r \geq 0, \tag{5.18}$$

where the angular brackets indicate the natural inner product on $\mathcal{W} \widehat{\bigotimes} \mathcal{W}$.

5.2 Theorem There exists a topological isomorphism

$$\kappa : \mathcal{W} \widehat{\bigotimes} \mathcal{W}[\nu \widehat{\otimes} \nu] \to \mathrm{T}[\alpha] \tag{5.19.a}$$

such that

$$\kappa(x \otimes y) w = \langle Jx, w \rangle y \qquad x, y, w \in \mathcal{W}, \tag{5.19.b}$$

and the duality between $\mathcal{W} \widehat{\bigotimes} \mathcal{W}$ and $\mathcal{L}^+(\mathcal{W})$ is translated in this isomorphism to the formula

$$[T, A] = \operatorname{tr}\left(\overline{A\, \kappa(T)}\right), \qquad T \in \mathcal{W} \widehat{\bigotimes} \mathcal{W},\ A \in \mathcal{L}^+(\mathcal{W}). \tag{5.20}$$

Proof For any $T \in \mathcal{W}\widehat{\bigotimes}\mathcal{W}$, consider the linear map $\overline{\kappa(T)}$ of $\mathcal{H}$ into $\mathcal{W}$ given by the formula

$$\overline{\kappa(T)}\xi = (j\xi \otimes I)(T), \qquad \xi \in \mathcal{H}.$$

Note that $j\xi \otimes I$ is an element of $\mathcal{L}\left(\mathcal{W}\widehat{\bigotimes}\mathcal{W}, \mathcal{W}\right)$, the tensor product of $j\xi \in \mathcal{W}'$ and $I \in \mathcal{L}(\mathcal{W})$.

If x, $y \in \mathcal{W}$ and ξ, $\eta \in \mathcal{H}$, it is simple to check that

$$\langle (j\xi \otimes I)(x \otimes y), \eta\rangle = \langle \xi, (j\eta \otimes I)(Jy \otimes Jx)\rangle.$$

Linearity and continuity then imply that

$$\langle \overline{\kappa(T)}\xi, \eta\rangle = \langle \xi, \overline{\kappa(T^*)}\eta\rangle, \qquad T \in \mathcal{W}\widehat{\bigotimes}\mathcal{W},\ \xi, \eta \in \mathcal{H}.$$

This proves that $\overline{\kappa(T)} \in \mathcal{L}(\mathcal{H})$, and its adjoint is given by

$$\left[\overline{\kappa(T)}\right]^* = \overline{\kappa(T^*)}.$$

We now write $\kappa(T)$ for the restriction of $\overline{\kappa(T)}$ to $\mathcal{W}$. We see that $\kappa(T) \in \mathcal{L}^+(\mathcal{W})$ and

$$\kappa(T)^+ = \kappa(T^*).$$

By this we see that we have defined a linear map κ from $\mathcal{W}\widehat{\bigotimes}\mathcal{W}$ to T.

Let

$$T = \sum\nolimits_{\mathbf{n},\mathbf{m}} \alpha_{\mathbf{n},\mathbf{m}} w_{\mathbf{m}} \otimes w_{\mathbf{n}}$$

be any element of $\mathcal{W}\widehat{\bigotimes}\mathcal{W}$. Then for any $r \geq 0$ and any $\mathbf{k}$ we have

$$M^r \kappa(T) M^r w_{\mathbf{k}} = \sum\nolimits_{\mathbf{n}} \alpha_{\mathbf{kn}} \|M^r w_{\mathbf{k}}\| M^r w_{\mathbf{n}},$$

so that

$$\|\kappa(T)\|_{2,r}{}' = \left\|\sum\nolimits_{\mathbf{n},\mathbf{m}} \alpha_{\mathbf{n},\mathbf{m}} M^r w_{\mathbf{m}} \otimes M^r w_{\mathbf{n}}\right\| = \|T\|_r{}''$$

for any $r \geq 0$.

If $R \in \mathrm{T}$, some algebraic rearrangement leads to

$$\|w_{\mathbf{n}} \otimes Rw_{\mathbf{n}}\|_r{}'' = \|M^r R M^r w_{\mathbf{n}}\| \leq \left\|M^{-1} w_{\mathbf{n}}\right\| \left\|M^{r+1} R M^{r+1} w_{\mathbf{n}}\right\|,$$

for all $\mathbf{n}$. It follows that

$$\sum\nolimits_{\mathbf{n}} \|w_{\mathbf{n}} \otimes Rw_{\mathbf{n}}\|_r{}'' \leq \left\|M^{-1}\right\|_2 \|R\|_{2,r+1}{}'.$$

Since this is true for all $r \geq 0$, it follows that

$$T_R = \sum_{n} w_n \otimes R w_n$$

converges in $\mathcal{W}\widehat{\bigotimes}\mathcal{W}$. It is easy to verify that

$$\kappa(T_R)x = Rx, \qquad \forall x \in \mathcal{W},$$

so that $\kappa(T_R) = R$. Thus κ is surjective, and so is the required topological isomorphism.

It also a simple matter to verify that

$$\mathrm{tr}\left(\overline{A\kappa(x \otimes y)}\right) = \langle Jx, Ay\rangle = [x \otimes y, A]$$

for all x, $y \in \mathcal{W}$ and all $A \in \mathcal{L}^+(\mathcal{W})$. Given A, choose an r so that M^{-r} is bounded. Then

$$\mathrm{tr}\left(\overline{A\kappa(T)}\right) \leq \|AM^{-r}\| \, \|M^{-r}\| \, \|\kappa(T)\|_{1,r}{}'$$

shows that the map $T \to \mathrm{tr}\left(\overline{A\kappa(T)}\right)$ is a continuous linear functional on $\mathcal{W}\widehat{\bigotimes}\mathcal{W}$. It follows that

$$[T, A] = \mathrm{tr}\left(\overline{A\kappa(T)}\right), \qquad T \in \mathcal{W}\widehat{\bigotimes}\mathcal{W},\ A \in \mathcal{L}^+(\mathcal{W}).$$

■

We now state the main result of this section. This is the theorem to which we have earlier referred, showing that all linear functionals on $\mathcal{A}$ are traces. This is one of the positive attributes of the model.

5.3 Corollary Every continuous functional T on $\mathcal{L}^+(\mathcal{W})$ can be identified with a trace class operator $\kappa(T) \in \mathrm{T}$, and conversely. The duality between $\mathcal{L}^+(\mathcal{W})$ and T is given by a trace,

$$T, A \to \mathrm{tr}\left(\overline{A\kappa(T)}\right). \tag{5.21}$$

The set of hermitian functionals may be identified as

$$\mathcal{L}^+(\mathcal{W})'_h \cong \{\, R \in \mathrm{T} : R = R^+ \,\} \tag{5.22}$$

The set of positive functionals may be identified as

$$\mathcal{L}^+(\mathcal{W})'_+ = \{\, R \in \mathrm{T} : R \geq 0 \,\}. \tag{5.23.a}$$

The set of states may be identified with

$$\mathrm{S} = \left\{ R \in \mathcal{L}^+(\mathcal{W})'_+ : \mathrm{tr}\left(\overline{R}\right) = 1 \right\}. \tag{5.23.b}$$

The relation between these sets is similar to that holding for general trace class operators:

$$\mathcal{L}^+(\mathcal{W})' = \mathcal{L}^+(\mathcal{W})'_h + i\,\mathcal{L}^+(\mathcal{W})'_h \tag{5.24.a}$$

$$\mathcal{L}^+(\mathcal{W})'_h = \mathcal{L}^+(\mathcal{W})'_+ - \mathcal{L}^+(\mathcal{W})'_+ \tag{5.24.b}$$

The set of states evidently form a base for the cone $\mathcal{L}^+(\mathcal{W})'_+$, which is generating. ■

We shall refer to elements of T as $\mathcal{W}$-nuclear operators. Similarly, we shall refer to hermitian and positive $\mathcal{W}$-nuclear operators. Elements of T corresponding to states will be known as $\mathcal{W}$-density matrices. Hereafter we drop the distinction between the various isomorphic spaces. Thus we sometimes refer to a density matrix as a state, and vice versa.

5.3 STATES AND REPRESENTATIONS

At the end of Chapter 3 we considered *–representations of locally convex algebras. We found there that the GNS construction related states to closed strongly cyclic *–representations. The extreme states correspond in this way to algebraically irreducible *–representations of this sort. We recall that for locally convex algebras in general, algebraic irreducibility does not imply that all vectors in the representation space are strongly cyclic. By way of example we noted that a smooth function of compact support is not cyclic for the polynomial algebra of the *ccr* in the Schrödinger representation. This example depends critically on the choice of the polynomial algebra. For the full algebra of observables $\mathcal{A}$, every vector in $\mathcal{W}$ is strongly cyclic, as we shall see.

We also recall that we have shown in Chapter 2 that all s–class representations of the *ccr* are equivalent. What we shall do now is to consider the GNS representation for states on the algebra $\mathcal{A}$ of observables, and note how the equivalence of s–class representations fits in to the general theory.

5.4 Proposition The GNS representation of $\mathcal{A}$ associated with a vector state T_x, where

$$T_x(a) = \langle x, ax\rangle, \qquad (x \in \mathcal{W},\, a \in \mathcal{A}). \tag{5.25}$$

is unitarily equivalent to the usual Schrödinger representation of $\mathcal{A}$ on $\mathcal{W}$. It is algebraically irreducible, and hence, the vector state T_x is pure.

Conversely, every pure state is a vector state.

Proof Since the left kernel is

$$L = \{ a \in \mathcal{A} : T_x(a^+ a) = 0 \}$$
$$= \{ a \in \mathcal{A} : ax = 0 \},$$

there is a linear bijection $\mathcal{A}/L \to \mathcal{A}\, x$ given by the map $a + L \to ax$. Indeed, this is an isometric isomorphism between the pre–Hilbert spaces $(\mathcal{A}/L, \langle \cdot, \cdot \rangle_{T_x})$ and $(\mathcal{A}\, x, \langle \cdot, \cdot \rangle)$.

For any y, $z \in \mathcal{W}$ consider $P_{y,z} \in \mathcal{L}(\mathcal{W})$ given by

$$P_{y,z}\, w = \langle y, w \rangle z, \qquad (w \in \mathcal{W}).$$

Clearly $P_{y,z} \in \mathcal{L}^+(\mathcal{W})$, as $P^+_{y,z} = P_{z,y}$. Since

$$P_{x,y} x = \|x\|^2\, y = y,$$

we deduce that $\mathcal{A}\, x = \mathcal{W}$.

Thus we have an isometric isomorphism from $(\mathcal{A}/L, \langle \cdot, \cdot \rangle_{T_x})$ to $(\mathcal{W}, \langle \cdot, \cdot \rangle)$ which intertwines the GNS action of $\mathcal{A}$ on $\mathcal{A}/L$ with the standard action of $\mathcal{A}$ on $\mathcal{W}$.

If $A \in \mathcal{L}(\mathcal{H})$ is such that

$$\langle Ax, ay \rangle = \langle a^+ x, A^* y \rangle$$

for all $a \in \mathcal{A}$ and x, $y \in \mathcal{W}$, then setting $x = w_n$, $y = w_m$ and $a = P_{w,z}$ gives

$$\langle w, w_n \rangle \langle A w_m, z \rangle = \langle w_m, z \rangle \langle A w, w_n \rangle.$$

Choosing first $w = z = w_m$ and $n \neq m$, and then $w = w_n$ and $z = w_m$ yields $A = cI$ for some constant $c \in \mathbb{C}$.

Thus the strong bounded commutant is trivial, and so the Schrödinger representation of $\mathcal{A}$ on $\mathcal{W}$ is algebraically irreducible. This implies that every vector state is pure.

We now show that every pure state is a vector state. Let T be a state and consider its tracial representation,

$$T(a) = \operatorname{tr}\left[\overline{a\kappa(T)}\right],$$

as in Corollary [5.3]. Moreover, it can be shown that there exists a sequence $r_n > 0$ of positive numbers which sum to unity, and an orthonormal family $e_n \in \mathcal{W}$ such that $\kappa(T) = \sum r_n P_{e_n, e_n}$, cf, Hennings [1]. Then

$$T(a) = \sum r_n \langle e_n, a e_n \rangle$$
$$= \sum r_n T_n(a),$$

defining the vector states T_n.

Now if and only if more than one r_n appears in the above sum, T is a nontrivial sum of other states. Then if T is pure, only one r_n occurs, and T is seen to be a vector state. ■

In view of the example noted above, concerning functions of compact support, this result is not true for the choice of $\mathcal{P}$ as the observable algebra. Put slightly differently, there is not always an operator in $\mathcal{P}$ which maps a vector $x \in \mathcal{W}$ to w_0. Sometimes there is, of course, as the equation

$$(n!)^{-1/2} b^n w_n = w_0$$

shows.

The following continuity results hold for the GNS representations.

5.5 Proposition By a weakly continuous representation of $\mathcal{A}$ we mean that

$$\mathcal{A} \to \mathbb{C};\ a \mapsto \langle y, \pi(a)x \rangle$$

is continuous for all x, $y \in D$. Every GNS representation of $\mathcal{A}$ is weakly continuous.

Proof Let $(\pi,\ D,\ v)$ be the GNS representation for the state T. Take $c \in \mathcal{A}$ to be an element of the equivalence class x, and similarly $d \in y$. Writing

$$\begin{aligned} F(a) &= \langle y, \pi(a)x \rangle \\ &= T(c^+ ad), \end{aligned}$$

F is continuous as the product on $\mathcal{A}$ is separately continuous. Hence the representation is weakly continuous. ■

5.4 ALGEBRAIC AND TOPOLOGICAL PROPERTIES OF $\mathcal{A}'$

We have identified the dual of $\mathcal{A}$ with $\mathcal{W}\widehat{\otimes}\mathcal{W}$, and with the set of those trace class operators we have called $\mathcal{W}$-nuclear operators. We continue our analysis of $\mathcal{A}'$ with a number of results which are interesting in themselves, and will prove important in the theory of measurements.

We begin by noting that the set of $\mathcal{W}$-nuclear operators is stable under the operator product. This enables us to turn $\mathcal{A}'$ into a *–algebra in a natural way.

5.6 Lemma The space T is a *–algebra , under the natural composition of maps and their involution. Thus

$$T_1 \times T_2(a) = \mathrm{tr}\,(\overline{\rho_1 \rho_2 a})\,, \tag{5.26.a}$$

and

$$\begin{aligned} T^+(a) &= \overline{T(a^+)} && (5.26.b) \\ &= \mathrm{tr}\left(\overline{\rho^+ a}\right). && (5.26.c) \end{aligned}$$

Mapping this structure into $\mathcal{W}\widehat{\otimes}\mathcal{W}$, we obtain the product structure

$$(x \otimes y)(w \otimes v) = \langle Jx, v\rangle \, w \otimes y, \qquad x, y, v, w \in \mathcal{W}$$

and the involution as defined above. ■

Note that we have introduced the physicist's convention of writing $\kappa(T)$ as ρ; the isomorphisms we have shown imply that this can lead to no errors. Hereafter, when we speak of $\mathcal{A}'$ as an algebra we mean the above operations. We shall write μ' for the strong dual topology on $\mathcal{A}'$. Its basic topological properties follow from the known properties of $\mathcal{W}$. As a topological algebra, $\mathcal{A}'$ is rather well behaved.

5.7 Proposition The algebra $\mathcal{A}'[\mu']$ is a nuclear Fréchet *–algebra . The positive cone $\mathcal{A}'_+$ is closed and normal, and has an empty interior. $\mathcal{A}'$ is Q and lmc, but not b*.

Proof The lmc properties follow from the obvious relations

$$\|T^+\|_{0,r}{}' = \|T\|_{0,r}{}' \tag{5.27.a}$$

and inserting the factor $M^r M^{-r}$ twice,

$$\|T_1 \times T_2\|_{0,r}{}' \leq \|T_1\|_{0,r}{}' \, \|T_2\|_{0,r}{}'. \tag{5.27.b}$$

To see that the positive cone is closed we note that $\|T\|_{0,0}{}'$ is the usual operator norm. As positivity of $\mathcal{W}$-nuclear operators is the usual positivity for operators, the result is immediate from that for $\mathcal{L}(\mathcal{H})$.

Employing the usual $M^r M^{-r}$ trick, it follows that

$$\|T^m\|_{0,r}{}' \leq \left(\|T\|_{0,r}{}'\right)^2 \left(\|T\|_0{}'\right)^{m-2}, \qquad (m \geq 2).$$

Hence

$$\lim_{m\to\infty} \left(\|T^m\|_{0,r}{}'\right)^{1/m} \leq \|T\|_0{}'.$$

This is true for all r, so the spectral radius satisfies

$$\nu(T) \leq \|T\|_{0,0}{}',$$

implying that $\mathcal{A}'$ is a Q-algebra.

Now $\mathcal{A}'$ is nuclear and Fréchet, so it is normable if and only if $\mathcal{W}\widehat{\otimes}\mathcal{W}$, hence $\mathcal{W}$, is finite dimensional. This is not the case here, so $\mathcal{A}'$ is not a C^*–algebra . As a Q b^*–algebra is automatically a C^*–algebra , we deduce that $\mathcal{A}'$ is not a b^*–algebra .

Consider the normality of the positive cone. For any pair of positive functionals,

$$\begin{aligned}\|T_1 + T_2\|_{0,r}{}' &= \sup\{\, \langle M^r x, (\rho_1 + \rho_2) M^r x\rangle : \|x\| = 1 \,\} \\ &\geq \sup\{\, \langle \rho_1 M^r x, \, M^r x\rangle : \|x\| = 1 \,\} \\ &= \|T_1\|_{0,r}{}'.\end{aligned}$$

Finally, the cone has an empty interior because $\mathcal{A}'$ is not normable. ■

Let us summarize what we have done in this chapter so far in the form of the fourth axiom. This is meant to replace and extend Axiom 4a above.

Axiom 4. The space $\mathcal{A}'[\mu']$ of continuous linear functionals on the algebra $\mathcal{A}$ of observables for the quantum system $\Sigma_{(\vec{N},\vec{t})}$ may be identified with $\mathcal{W}[\nu]\widehat{\bigotimes}\mathcal{W}[\nu]$. It is isomorphic to the set T of $\mathcal{W}$-nuclear operators, the duality with $\mathcal{A}$ being given by the trace. The set $\mathcal{A}'_+$ of $\mathcal{K}$-positive linear functionals is a closed normal generating cone with empty interior. The set S of states consists of the positive functionals satisfying the normalization condition

$$T(\mathbf{1}) = 1.$$

$\mathcal{A}'_+$ may be identified with the positive $\mathcal{W}$-nuclear operators. The states then consist of positive $\mathcal{W}$-nuclear operators satisfying $\mathrm{tr}(\rho) = 1$, known as $\mathcal{W}$-density matrices. $\mathcal{A}'$ is a nuclear Fréchet *–algebra under the operations of multiplying and taking adjoints of density matrices. Hence it is barreled, bornological, Mackey, Montel, reflexive, and separable. It is lmc and Q, but not b*. The density matrix representation affords a decomposition of states into vector states. The vector states constitute the extreme points of the set of states; hence they are known as pure states. The GNS representation for a pure state is unitarily equivalent to the Schrödinger representation, and is closed, algebraically irreducible, self adjoint, and s–class. ∎

5.5 POSITIVITY PRESERVING MAPS

It is important for the physical interpretation of the theory to understand the nature of maps from $\mathcal{A}'$ to itself which preserve the positive cone $\mathcal{A}'_+$. We refer to such maps as positive. We shall employ the usual notation $L(X)$ and $\mathcal{L}(X)$ for the sets of all linear and all continuous linear maps from X to itself. The subscript + will indicate positivity preservation. That is, if X is an ordered vector space with positive cone C, then those maps in $L(X)$ which map C into itself constitute the wedge $L_+(X)$. Similarly for continuous maps, $\mathcal{L}_+(X)$.

There is a basic result for positive maps on $\mathcal{A}$ and $\mathcal{A}'$, stemming from the fact that μ is the order topology on $\mathcal{A}$.

5.8 Proposition Positive maps of $\mathcal{A}$ or $\mathcal{A}'$ to themselves are automatically continuous:

$$L_+(\mathcal{A}) = \mathcal{L}_+(\mathcal{A}), \tag{5.28.a}$$

and

$$L_+(\mathcal{A}') = \mathcal{L}_+(\mathcal{A}'). \tag{5.28.b}$$

Proof Every positive map on $\mathcal{A}$ is order bounded Peressini [1],Def 1.2.1, and every order bounded linear map between ordered vector spaces equipped with their order topologies is continuous, ibid 3.1.14. This proves equation (5.28.a) . As the cone in $\mathcal{A}$ is normal, the dual cone in $\mathcal{A}'$ is generating.

We now know that $\mathcal{A}'$ is a Fréchet space with a generating normal positive cone which is closed, hence complete. The Nachbin, Namioka, Schaeffer theorem, ibid 2.2.16.c, then asserts that every positive map is continuous, which is equation (5.28.b) , and we are done. ■

The material that follows is rather technical and concerns the convergence of certain families of maps on $\mathcal{A}'$. The reason is that an elementary quantum measurement can be identified with a certain sort of linear map between states. One then wants less elementary measurements to be limits of the simpler ones, and the results that follow enable such an approximation scheme to be set up.

We need the following terminology, due to Wright [1].

5.9 Definition An ordered vector space E is said to be monotone σ-complete if, whenever any monotone sequence (x_n) in E is bounded above in E, then it has a least upper bound in E, which we write as $\vee x_n$.

E is said to be monotone complete if every upward filtering subset $F \subset E$ with an upper bound has a least upper bound, denoted $\bigvee F$. ■

5.10 Proposition $\mathcal{A}'$ is monotone complete, hence monotone σ-complete.

Proof Schaeffer shows, [1],V.4.3, Cor 2, that a semi reflexive ordered locally convex space with closed normal positive cone is monotone complete. ■

The $\mathcal{W}$-nuclear operator representation of $\mathcal{A}'$ has led us to the spectral decomposition for these operators. We now establish a convergence result for this decomposition.

5.11 Proposition Let ρ be a positive $\mathcal{W}$-nuclear operator, and $\sum r_n P_{e_n,e_n}$ its spectral decomposition. Write ρ_N for the N-th partial sum. Then ρ_N converges to ρ in the uniform operator norm, the trace norm, and the μ' topology.

Proof Clearly

$$\operatorname{tr}(\rho - \rho_N) = \sum\nolimits_{j>N} r_j$$

converges to zero, as Lidskii's theorem says that (Simon [2])

$$\operatorname{tr}(\rho) = \sum_{j\geq 1} r_j.$$

As the trace norm dominates the operator norm, the first two statements have been shown.

Consider the convergence in the μ' topology. Now

$$\begin{aligned}\|M^r(\rho-\rho_N)M^r\| &\leq \operatorname{tr}([\rho-\rho_N]M^{2r}) \\ &= \sum_{j>N} r_j\,\|M^r e_j\|^2.\end{aligned}$$

As ρ is a positive $\mathcal{W}$-nuclear operator, the convergence to zero of this last expression is immediate. ■

In what follows, the subscript σ will indicate the topology of pointwise convergence, or the simple topology, on the relevant space of linear maps.

5.12 Proposition (a) The simple completion of the space of continuous maps on $\mathcal{A}'$ is the space of all maps:

$$\sigma - \text{completion}\,\mathcal{L}(\mathcal{A}'[\mu'])_\sigma = L(\mathcal{A}'[\mu'])_\sigma. \tag{5.29.a}$$

(b) $L(\mathcal{A}'[\mu'])_\sigma$ and $\mathcal{L}(\mathcal{A}'[\mu'])_\sigma$ are nuclear and semi reflexive spaces.

(c) Positive operators are necessarily continuous, in the sense that

$$L_+(\mathcal{A}'[\mu'])_\sigma = \mathcal{L}_+(\mathcal{A}'[\mu'])_\sigma. \tag{5.29.b}$$

(f) $\mathcal{L}_+(\mathcal{A}'[\mu'])_\sigma$ is a proper complete cone.

Proof Let E be a complete locally convex space. It is standard that

$$\mathcal{L}(E)_\sigma \subset \sigma - \text{completion}\,\mathcal{L}(E)_\sigma = L(E) \subset E^E.$$

If E is nuclear and semi reflexive, so is E^E. These properties are inherited by subspaces, and so (a) and (b) are true.

Peressini states ([1], §4.3) that if (E, C) and (F, D) are ordered topological vector spaces, and if the linear hull of $C - C$ is dense in E, then the positive wedge in $\mathcal{L}(E, F)$ is a proper cone. This is the case for E and F equal to $\mathcal{A}'$. The remaining properties are a consequence of $\mathcal{L}_+(\mathcal{A}'[\mu'])_\sigma$ being a closed subset of $\mathcal{L}(\mathcal{A}'[\mu'])_\sigma$, hence of $L(\mathcal{A}'[\mu'])_\sigma$. ■

The set of positive maps on $\mathcal{A}'$ satisfies a certain monotone convergence property.

5.13 Proposition If (u_ι) is an upper bounded and upward directed net in the cone $\mathcal{L}_+ (\mathcal{A}'_h[\mu'])_\sigma$, it converges in the simple topology to its supremum:

$$\sigma - \lim_\iota u_\iota = \sup_\iota u_\iota. \tag{5.30}$$

Proof The result is true because $\mathcal{L}_+ (\mathcal{A}'_h[\mu'])_\sigma$ is complete, and $\mathcal{A}'_h[\mu']$ is monotone complete. ∎

5.6 GENERALIZED EIGENVECTORS AND DIRAC'S NOTATION

The characteristic feature of spectral theory in infinite dimensional spaces is the presence of the continuous spectrum, first discovered by Hilbert [1] in 1906, in connection with his theory of integral equations. In the early formulation of the spectral theory of self adjoint operators in Hilbert spaces, due independently to Lorch, Stone and von Neumann, the central concept is that of a projection valued measure. This approach was extended to symmetric operators by Naimark. Naimark's theory requires the replacement of projection valued measures by positive operator valued measures.

Spectral theory is the principal tool in the quantum theory of measurements. As usually discussed, matters are based on eigenvectors and, even more, the assumption of an orthonormal basis of eigenvectors. For most observables this is completely untenable. The position and momentum operators, for example, have no eigenvectors at all. This does not signal any breakdown of the theory as such. Eigenvectors, if there are any, correspond to bound states, as we have noted before. The continuous spectrum corresponds to the scattering regime. Rather complex motion is represented here. For example, fragments of the system may separate off for a while and then recombine. The dissolution of a salt in water is a good example.

The consequence of this is that we must adapt the description of measurements to take these facts into account. For the bounded model, this has been done, eg, by Davies and Lewis [1], and Davies [1-2]. In Chapter 7 we shall present the variant necessary for the unbounded model.

At this point we shall introduce the spectral theory which we employ there. This spectral theory can be cast either into an operator or a distributional framework. In the distributional form it provides some insight into the rigged Hilbert space structure. In addition, distributions are necessary to discuss the Dirac bra and ket formalism. We do not use this formalism elsewhere, but it is of sufficient interest to physicists to make its inclusion into our model worthwhile.

We shall assume that the reader is familiar with the spectral theory for unbounded self adjoint operators. We present this in two forms. One is the projection valued measure form of Lorch and von Neumann. The second is in the Fourier transform form; these are completely equivalent. We shall write the two forms of the basic theorem down, so as to establish notation for what follows.

This theory does not apply to our model as it stands, as observables are generally hermitian but not self adjoint. Naimark has created a spectral theory for general symmetric operators. This requires extending the operators to Hilbert spaces containing the original Hilbert space. On these extended spaces, the extended operators have equal deficiency indices, and therefore self adjoint extensions. By projecting the spectral decompositions of these extensions back to the original space, the original operator may be represented as an integral over a spectral family of positive bounded operators. Unlike the self adjoint case, these operators are only positive, not projections. They do satisfy σ-additivity, however, and so are known as positive operator valued measures (POVM), as opposed to projection valued measures (PVM). Moreover, a given symmetric operator has many such representations, in general. In contrast, a self adjoint operator has a unique decomposition, up to unitary isomorphism. This extended spectral theory also has two forms, POVM and Fourier transform.

We remark that the full Naimark theorem constructs extensions of *-semigroups of operators. It also proves that there is a minimal extension in a certain sense, but these points are not necessary here. A full account may be found in Riesz and Sz.-Nagy [1].

We shall only need a particular form of Naimark's theory. As all the other spectral theory is completely standard, it seems reasonable to omit the proofs of all but an outline for this variant of Naimark's theorem.

After that we shall apply the theory to the algebra of observables. For this we must reconsider the spectral theory in the rigged Hilbert framework. This has been done by Gel'fand, Maurin and others, and a satisfactory theory turns out to be possible.

There are a great many references to these various aspects of spectral theory. We mention only those of Gel'fand and Vilenkin [1], Kato [1], Maurin [1], Reed and Simon [1], Riesz and Sz.-Nagy [1], and Yosida [1].

As a matter of notation, we shall write

$$L^{\omega}(\Lambda, d\mu) = \bigcap_{p\geq 1} L^{p}(\Lambda, d\mu).$$

As a matter of terminology, we shall refer to a countable family of mutually disjoint Borel subsets as a σ-family.

We start by setting down the definition of the sorts of spectral measures we shall use.

5.14 Definition (a) A spectral family, or resolution of the identity, on a Hilbert space $\mathcal{H}$, is a one parameter family of of projection operators,

$$\{ E_t : t \in \mathbb{R},\ 0 \leq E_t \leq I \},$$

satisfying the conditions

$$\mathcal{H} - \lim_{t \to -\infty} E_t x = 0; \tag{5.31.a}$$

$$\mathcal{H} - \lim_{t \to +\infty} E_t x = x; \tag{5.31.b}$$

$$\mathcal{H} - \lim_{\epsilon \to +0} E_{t-\epsilon} x = E_t x; \tag{5.31.c}$$

$$E_t E_s = E_{\min(s,t)}, \tag{5.31.d}$$

for all $x \in \mathcal{H}$.

(b) A generalized spectral family on a Hilbert space $\mathcal{H}$ is a one parameter family of positive contraction operators,

$$\{ B_t : t \in \mathbb{R},\ 0 \leq B_t \leq I \},$$

satisfying the conditions

$$\mathcal{H} - \lim_{t \to -\infty} B_t x = 0; \tag{5.32.a}$$

$$\mathcal{H} - \lim_{t \to +\infty} B_t x = x; \tag{5.32.b}$$

$$\mathcal{H} - \lim_{\epsilon \to +0} B_{t-\epsilon} x = B_t x; \tag{5.32.c}$$

$$B_t \leq B_s, \quad t \leq s, \tag{5.32.d}$$

for all $x \in \mathcal{H}$.

(c) A projection valued measure (PVM) is a family,

$$\mathcal{E} : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})_+ ,$$

of maps from the Borel subsets of $\mathbb{R}$ into the projection operators on $\mathcal{H}$, satisfying

$$\mathcal{E}_{\emptyset} = 0; \tag{5.33.a}$$

$$\mathcal{E}_{\mathbb{R}} = I; \tag{5.33.b}$$

$$\mathcal{E}_{\Delta_1} \mathcal{E}_{\Delta_2} = \mathcal{E}_{\Delta_1 \cap \Delta_2}; \tag{5.33.c}$$

$$\mathcal{E}_{\bigcup \Delta_j} x = \mathcal{H} - \lim_{n \to \infty} \sum_{j \leq n} \mathcal{E}_{\Delta_j} x, \tag{5.33.d}$$

for all $x \in \mathcal{H}$ and every σ-family. This last property is known as strong σ-additivity.

Spectral families and projection valued measures are in one-one correspondence through the equation

$$E_t = \mathcal{E}_{(-\infty,t)}. \tag{5.33.e}$$

(d) A positive operator valued measure (POVM) is a family,

$$\mathcal{B} : \mathrm{Bor}\,(\mathbb{R}) \to \mathcal{L}\,(\mathcal{H})_+ \,,$$

of maps from the Borel subsets of $\mathbb{R}$ into the positive bounded operators on $\mathcal{H}$, satisfying

$$\mathcal{B}_{\emptyset} = 0; \tag{5.34.a}$$

$$\mathcal{B}_{\mathbb{R}} = I; \tag{5.34.b}$$

$$\mathcal{B}_{\Delta_1} \leq \mathcal{B}_{\Delta_2}, \qquad \Delta_1 \subseteq \Delta_2; \tag{5.34.c}$$

$$\mathcal{B}_{\bigcup \Delta_j} x = \mathcal{H} - \lim_{n\to\infty} \sum\nolimits_{j\leq n} \mathcal{B}_{\Delta_j} x, \tag{5.34.d}$$

for all $x \in \mathcal{H}$ and every σ-family.

Generalized spectral families and positive operator valued measures are in one-one correspondence through the equation

$$B_t = \mathcal{B}_{(-\infty,t)}. \tag{5.34.e}$$

(e) A contraction operator valued measure (COVM) is a family,

$$\mathcal{C} : \mathrm{Bor}\,(\mathbb{R}) \to \mathcal{L}\,(\mathcal{H})\,,$$

of maps from the Borel subsets of $\mathbb{R}$ into the contraction operators on $\mathcal{H}$, satisfying strong σ-additivity. ■

This next theorem provides the spectral decomposition theory for self adjoint operators. Our terminology is borrowed from Maurin [1].

5.15 The Complete Spectral Theorem (a) **Fourier Transforms.** Let A be a self adjoint operator on a Hilbert space $\mathcal{H}$, with domain $D(A)$. There exists
(i) a locally compact separable measure space Λ, and a finite positive Borel measure (Λ, μ) on it;
(ii) a μ–measurable field $(\widetilde{\mathcal{H}}_\lambda)_{\lambda\in\Lambda}$ of Hilbert spaces, with corresponding dimensions

$$\dim \widetilde{\mathcal{H}}_\lambda = d(\lambda), \tag{5.35.a}$$

whose direct integral we denote by

$$\widetilde{\mathcal{H}} = \int_{\Lambda}^{\oplus} \widetilde{\mathcal{H}}_{\lambda}\, d\mu(\lambda); \tag{5.35.b}$$

(iii) a decomposition of each $\widetilde{\mathcal{H}}_{\lambda}$ into one dimensional component Hilbert spaces,

$$\widetilde{\mathcal{H}}_{\lambda} = \sum_{k=1}^{d(\lambda)}{}^{\oplus}\, \widetilde{\mathcal{H}}_{k,\lambda}; \tag{5.36}$$

(iv) and a unitary transformation

$$\mathcal{F} : \mathcal{H} \to \widetilde{\mathcal{H}} \tag{5.37}$$

onto the direct integral of the above fields.

We shall write $\mathcal{F}(u)$ or $\widetilde{u}$ as is convenient. Similarly, we write $\mathcal{F}A\mathcal{F}^{-1}$ as $\widetilde{A}$.

The decomposition may be written either in terms of vectors in $\widetilde{\mathcal{H}}_{\lambda}$ or in terms of the one dimensional components in $\widetilde{\mathcal{H}}_{k,\lambda}$. Thus,

$$\widetilde{\mathcal{H}} = \int_{\Lambda}^{\oplus} \sum_{k=1}^{d(\lambda)}{}^{\oplus}\, \widetilde{\mathcal{H}}_{k,\lambda}\, d\mu(\lambda) \tag{5.38}$$

for the Hilbert space. For the components,

$$\begin{aligned} \mathcal{F}(u) &= \widetilde{u} \\ &= \int_{\Lambda}^{\oplus} \widetilde{u}_{\lambda}\, d\mu(\lambda) && (5.39.a) \\ &= \int_{\Lambda}^{\oplus} \sum_{k=1}^{d(\lambda)}{}^{\oplus}\, \widetilde{u}_{k,\lambda}\, d\mu(\lambda). && (5.39.b) \end{aligned}$$

The map $\mathcal{F}$ diagonalizes the operator A, so that $\widetilde{A}$ is a multiplication operator. That is, there exists a spectral function $F \in L^{\omega}(\Lambda, d\mu)$ which yields the spectrum of A as its range :

$$\mathrm{Sp}(A) = \{\, F(\lambda) : \lambda \in \Lambda \,\}; \tag{5.40}$$

and such that for all $u \in D(A)$,

$$\begin{aligned} \mathcal{F}(Au) &= \widetilde{A}\widetilde{u} \\ &= \int_{\Lambda}^{\oplus} F(\lambda)\widetilde{u}_{\lambda}\, d\mu(\lambda) && (5.41.a) \\ &= \int_{\Lambda}^{\oplus} F(\lambda) \sum_{k=1}^{d(\lambda)}{}^{\oplus}\, \widetilde{u}_{k,\lambda}\, d\mu(\lambda). && (5.41.b) \end{aligned}$$

The inner product on $\widetilde{\mathcal{H}}$ is given by

$$\langle \widetilde{u}, \widetilde{v} \rangle = \int_\Lambda \langle \widetilde{u}_\lambda, \widetilde{v}_\lambda \rangle \, d\mu(\lambda) \tag{5.42.a}$$

$$= \int_\Lambda \sum_{k=1}^{d(\lambda)} \langle \widetilde{u}_{k,\lambda}, \widetilde{v}_{k,\lambda} \rangle \, d\mu(\lambda). \tag{5.42.b}$$

The unitary map $\mathcal{F}$ is known as the (generalized) Fourier transform. This is because if A is the momentum operator in one dimension, the $\widetilde{u}_{k,\lambda}$ are the classical Fourier components.

As each $\widetilde{\mathcal{H}}_{k,\lambda}$ is one dimensional, there is a unitary isomorphism from $\widetilde{\mathcal{H}}_{k,\lambda}$ onto $\mathbb{C}$. We write $\widehat{u}_{k,\lambda}$ for the image of $\widetilde{u}_{k,\lambda}$ under this isomorphism. This distinction will help clarify matters below. With this notation we can rewrite the inner product as

$$\langle \widetilde{u}, \widetilde{v} \rangle = \int_\Lambda \sum_{k=1}^{d(\lambda)} \widehat{u}^*_{k,\lambda} \, \widehat{v}_{k,\lambda} \, d\mu(\lambda). \tag{5.42.c}$$

(b) **PVM Form.** Let $\mathcal{M}$ be the W^*–algebra subalgebra of $\mathcal{L}(\mathcal{H})$ generated by the Cayley transform of A, and write $B_b(\mathbb{R})$ for the bounded Borel functions on $\mathbb{R}$. There exists a W^*-homomorphism Ψ from $B_b(\mathbb{R})$ into $\mathcal{M}$ such that

$$\mathcal{F}\left[\Psi(f)u\right](\lambda) = f \circ F(\lambda)\widetilde{u}(\lambda), \qquad u \in \mathcal{H}, \; \mu - ae. \tag{5.43}$$

If we define $E : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ by

$$E_\Delta = \Psi(\kappa_\Delta), \tag{5.44}$$

where κ_Δ is the characteristic function of the Borel set Δ, then E is a projection valued measure. The map Ψ extends to all real valued Borel functions, not necessarily bounded, such that

$$D\left[g(A)\right] = \left\{ u \in \mathcal{H} : \int_{\mathbb{R}} |g(t)|^2 \, d\langle u, E_t u \rangle < \infty \right\},$$

$$g(A) = \int_{\mathbb{R}} g(t) \, E(dt). \tag{5.45.a}$$

In particular,

$$A = \int_{\mathbb{R}} t \, E(dt). \tag{5.45.b}$$

■

As noted above, it will be necessary for us to use the Naimark extended spectral theory.

5.16 Naimark Spectral Theorem If $A : D \to \mathcal{H}$ is a closed densely defined symmetric operator, a spectral function for A is a POVM

$$\mathcal{B} : \mathrm{Bor}\,(\mathbb{R}) \to \mathcal{L}\,(\mathcal{H})_+$$

such that

$$\langle x, Ay \rangle = \int_{\mathbb{R}} t\, d\langle x, B_t y \rangle, \qquad x \in \mathcal{H},\ y \in D, \tag{5.46.a}$$

and

$$\|Ay\|^2 = \int_{\mathbb{R}} t^2\, d\langle y, B_t y \rangle, \qquad y \in D. \tag{5.46.b}$$

The preceeding comments show that any self adjoint operator possesses a spectral function E which is a PVM. Moreover, for any $y \in D$ and $s \geq 0$, $\int_{-s}^{s} t\, E(dt)\, y$ is a well defined element of $\mathcal{H}$. It can then be shown that as $s \to \infty$, these elements converge to Ay in $\mathcal{H}$.

Any closed symmetric densely defined operator $A : D \to \mathcal{H}$ possesses a spectral function. This spectral function is unique, up to unitary equivalence, if and only if A is maximal symmetric. This unique spectral function is a PVM if and only if A is self adjoint.

As a purely symbolic notation for (5.46.a-b), it is often convenient to write

$$A = \int_{\mathbb{R}} t\, \mathcal{B}(dt). \tag{5.46.c}$$

Not all POVM are spectral functions, since the set of u for which (5.46.b) holds can consist of the zero vector alone.

In particular, one POVM for any closed symmetric operator may be obtained as follows. Consider the operator $A \bigoplus -A$ defined on the domain $D \bigoplus D$ in the extension Hilbert space $\mathcal{H} \bigoplus \mathcal{H}$. This operator has a certain self adjoint extension $\widetilde{A}$, and corresponding PVM E, POVM $\mathcal{B}$ and COVM $\mathcal{D}$, such that: E is the unique PVM associated to $\widetilde{A}$ by (5.45.b); and satisfies the decomposition rule

$$E_\Delta(x \oplus y) = [\mathcal{B}_\Delta x + \mathcal{D}_{-\Delta} y] \oplus [\mathcal{D}_\Delta x + \mathcal{B}_{-\Delta} y], \qquad x, y \in \mathcal{H},\ \Delta \in \mathrm{Bor}\,(\mathbb{R}). \tag{5.47}$$

Apply the Fourier transform form of the spectral theorem to $\widetilde{A}$, so that

$$\mathcal{F} : \mathcal{H} \bigoplus \mathcal{H} \to L^2\,(M,\, d\mu)$$

diagonalizes it, with spectral function F so that

$$[\mathcal{F}\,(E_\Delta X)]\,(\lambda) = \kappa_\Delta \circ F(\lambda)\,(\mathcal{F} X)\,(\lambda), \qquad X \in \mathcal{H},\ \mu - ae. \tag{5.48}$$

The adjoint relations of the associated operator valued measures are

$$\mathcal{B}_\Delta^* = \mathcal{B}_\Delta, \tag{5.49.a}$$

$$\mathcal{D}_\Delta^* = \mathcal{D}_{-\Delta}. \tag{5.49.b}$$

They satisfy the product relations

$$\mathcal{B}_\Delta \mathcal{B}_{\Delta'} = \mathcal{B}_{\Delta\cap\Delta'} - \mathcal{D}_{-\Delta}\mathcal{D}_{\Delta'}, \tag{5.50.a}$$

$$\mathcal{D}_\Delta \mathcal{B}_{\Delta'} = \mathcal{D}_{\Delta\cap\Delta'} - \mathcal{B}_{-\Delta}\mathcal{D}_{\Delta'}, \tag{5.50.b}$$

for all Δ, $\Delta' \in \operatorname{Bor}(\mathbb{R})$.

The COVM $\mathcal{D}$ vanishes if and only if A is self adjoint.

Proof The operator $A \bigoplus -A$ has equal deficiency indices. The particular self adjoint extension in question is obtained by extending its Cayley transform to act as

$$x \oplus y \mapsto y \oplus x$$

from $\operatorname{ran}([A \bigoplus -A] + i)^\perp$ to $\operatorname{ran}([A \bigoplus -A] - i)^\perp$. This extension V is unitary, and so must be the Cayley transform of a self adjoint operator, which we denote $\widetilde{A}$.

We apply the complete spectral theorem to $\widetilde{A}$, and this determines $(\Lambda, d\mu)$, $\mathcal{F}$, F and the PVM E.

The next step is crucial. We set

$$E_\Delta(x \oplus 0) = \mathcal{B}_\Delta x \oplus \mathcal{D}_\Delta x \tag{5.51}$$

and seek the properties of $\mathcal{B}$ and $\mathcal{D}$.

By taking the inner product of (5.51) with $x \oplus 0$ we see that

$$\langle x, \mathcal{B}_\Delta x\rangle = \langle x \oplus 0, E_\Delta x \oplus 0\rangle,$$

and so $\mathcal{B}_\Delta$ is positive.

By taking the inner product of (5.51) with itself, we get

$$\begin{aligned}\|\mathcal{B}_\Delta x\|^2 + \|\mathcal{D}_\Delta x\|^2 &= \|E_\Delta x\|^2 \\ &\leq \|x\|^2.\end{aligned}$$

Hence $\mathcal{B}_\Delta$ and $\mathcal{D}_\Delta$ are contractions.

The strong σ-additivity follows from that of E and the continuity of the projections P and $I - P$ onto the first and second components of $\mathcal{H} \bigoplus \mathcal{H}$. Hence $\mathcal{B}$ is a POVM and $\mathcal{D}$ a COVM.

By acting on (5.51) with P we get

$$PE_\Delta(x \oplus 0) = \mathcal{B}_\Delta x. \tag{5.52.a}$$

As

$$P\widetilde{A}(x \oplus 0) = Ax, \tag{5.52.b}$$

it follows that (5.46) holds.

Consider the reversal operator

$$C(x \oplus y) = (y \oplus x) \tag{5.53.a}$$

on $\mathcal{H} \bigoplus \mathcal{H}$. It is easy to show that it almost intertwines V, in the sense that

$$CV = V^*C. \tag{5.53.b}$$

This enables us to apply the Fourier transform to $C\widetilde{A}C$ and show that

$$CE_\Delta C = E_{-\Delta}. \tag{5.53.c}$$

The point of this is to obtain information about the action of E on the second component. With the previous equation, the basic result (5.47) is immediate. We are also able to obtain the action of $\mathcal{D}$ on $\mathcal{H}$ by action with $I - P$:

$$(I - P)E_\Delta(0 \oplus x) = \mathcal{D}_\Delta x. \tag{5.54}$$

The adjoint and product relations follow directly from (5.47) by direct calculation.

The question of self adjointness is shown simply. If $\mathcal{D}$ is the zero measure, the product relation for $\mathcal{B}$ shows that it is then a PVM, so A is self adjoint.

Conversely, suppose A is self adjoint. Thus the Cayley transform of $A \bigoplus -A$ is unitary. Then $\mathcal{H} \bigoplus \{0\}$ is invariant under it, and so it commutes with $\mathcal{P}$. Then P commutes with the E_Δ, which imples that $\mathcal{D}$ is the zero measure.

Uniqueness and the PVM property follows for maximal and self adjoint operators, respectively, from the theory of generalized resolvents, and we refer to Akhiezer and Glazman [1], Volume II, § 112, Theorem 2 for a proof. ■

In the case of a rigged Hilbert space, the above spectral theorems take a particularly interesting form. We shall start with the simplest case of an operator with equal deficiency indices. This is the content of Maurin's nuclear spectral theorem, which finds applications not only in quantum mechanics, but in quantum field theory and the representation theory of Lie groups (Maurin [1–3]). We note that our name for this theorem is not standard; Maurin refers to it as the fundamental theorem ([1], XVII, 1). We refer the reader there for other applications.

5.17 Maurin's Nuclear Spectral Theorem Let

$$\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi' \tag{5.55}$$

be a rigged Hilbert space, where Φ is a Fréchet nuclear space, and let $a \in \mathcal{L}^+(\Phi)$ be symmetric and have equal deficiency indices. Then there exist elements $(\widetilde{T}_{k,\lambda} \in \Phi')_{k,\lambda}$ which are generalized eigenvectors of a and determine the Fourier coefficients. That is,

$$\widetilde{T}_{k,\lambda}(au) = F(\lambda)\widetilde{T}_{k,\lambda}(u), \qquad u \in \Phi, \tag{5.56}$$

for μ–almost all λ, which is the definition of a generalized eigenfunction. The Fourier coefficients are given by

$$\widehat{u}_{k,\lambda} = \widetilde{T}_{k,\lambda}(u), \qquad u \in \Phi, \tag{5.57}$$

for μ–almost all λ.

If we do not wish to decompose the $\widetilde{\mathcal{H}}_\lambda$ into one dimensional components, then

$$T_\lambda(u) = \widetilde{u}_\lambda \tag{5.58}$$

defines maps in $\mathcal{L}\left(\Phi, \widetilde{\mathcal{H}}_\lambda\right)$ for μ-almost all λ. These are vector valued generalized eigenvectors, in the sense of Gel'fand and Vilenkin [1].

If

$$\widetilde{T}_{k,\lambda}(u) = 0, \qquad u \in \Phi, \mu - ae, \tag{5.59}$$

then $u = 0$. Gel'fand and Vilenkin [1] refer to this as a having a complete set of generalized eigenvectors.

Proof As a has equal deficiency indices, we may choose a self adjoint extension, say $A : D \to \mathcal{H}$. The fundamental theorem of Maurin (ibid) yields (5.41) and (5.42) for any subspace E of D which is stable under A and such that $(E, \mathcal{H}, E')$ is a rigged Hilbert space. This is true for $E = \Phi$. As A restricted to Φ is a, the first part of the theorem is true.

The completeness of the system of eigenvectors is also reasonably obvious. For (5.59) implies that

$$\|\widetilde{u}\|^2 = 0,$$

and $\mathcal{F}$ is unitary.

It remains to prove Maurin's fundamental theorem. By assumption, E may be represented as the inductive limit of a countable family (E_n) of Hilbert spaces such that the embedding maps

$$J_n : E_n \to E$$

are Hilbert-Schmidt class (HS). Thus, there exists an orthonormal basis $\left(e_j^n\right)_j$ for E_n and a countable family $\left(h_j^n\right)_j \subset E_n$ for which

$$\sum\nolimits_j \left\|h_j^n\right\|^2 < \infty,$$

and such that

$$J_n(u_n) = \sum\nolimits_j \langle e_j^n, u_n\rangle h_j^n.$$

As the Fourier transform is unitary,

$$\sum\nolimits_j \left\|\mathcal{F}h_j^n\right\|^2 < \infty,$$

and so $\mathcal{F} \circ J_n$ is HS-class.

Fubini's theorem then gives

$$\int_\Lambda \sum\nolimits_j \left\|\mathcal{F}h_j^n(\lambda)\right\|^2 d\mu(\lambda) < \infty.$$

Hence

$$\sum\nolimits_j \left\|\mathcal{F}h_j^n(\lambda)\right\|^2 < \infty$$

for μ-almost all λ, and so the maps

$$u_n \mapsto (\mathcal{F}u_n)(\lambda), \qquad u_n \in E_n,$$

are HS-class for μ-almost all λ and all n.

By nuclearity, the maps

$$u \mapsto (\mathcal{F}u)(\lambda), \qquad u \in E,$$

are continuous for μ-almost all λ. Thus μ-almost all the $\widetilde{\mathcal{H}}_\lambda$ valued maps T_λ are continuous. Similarly for the components taking values in $\widetilde{\mathcal{H}}_{k,\lambda}$. Going over from $\widetilde{\mathcal{H}}_{k,\lambda}$ to $\mathbb{C}$, we find that $\widetilde{T}_{k,\lambda} \in E'$ for μ-almost all λ. ∎

We can now combine the results above to show that every hermitian observable has a complete set of generalized eigenfunctions.

5.18 Corollary Let $a \in \mathcal{L}^+(\mathcal{W})_h$ be hermitian, $a^+ = a$, but not necessarily essentially self adjoint. There exists a measure space (Λ, μ) as in [5.15] above, and a complete family

$$\left\{ \widetilde{T}_{k,\lambda} \in \mathcal{W}' : 1 \leq k \leq d(\lambda),\, \lambda \in \Lambda \right\}$$

of generalized eigenvectors for a:

$$\widetilde{T}_{k,\lambda}(au) = F(\lambda)\widetilde{T}_{k,\lambda}(u), \qquad u \in \mathcal{W}. \tag{5.60}$$

Proof We double up, and consider $a \oplus -a \in \mathcal{W} \bigoplus \mathcal{W}$ which has the particular self adjoint extension described in [5.16].

As the direct sum of two spaces preserves the rigged Hilbert structure,

$$\mathcal{W} \bigoplus \mathcal{W} \hookrightarrow \mathcal{H} \bigoplus \mathcal{H} \hookrightarrow \mathcal{W}' \bigoplus \mathcal{W}'$$

is a rigged triple. Moreover, $\mathcal{W} \bigoplus \mathcal{W}$ is a Fréchet nuclear space, and so we are assured of the existence of a complete family of distributions $\left\{ \widetilde{S}_{k,\lambda} \in \mathcal{W}' \bigoplus \mathcal{W}' : 1 \leq k \leq d(\lambda),\ \lambda \in \Lambda \right\}$ satisfying the eigenvalue equation

$$\widetilde{S}_{k,\lambda}[\widetilde{A}(u \oplus v)] = F(\lambda)\widetilde{S}_{k,\lambda}(u \oplus v), \qquad u, v \in \mathcal{W}.$$

For brevity we shall omit the proviso μ-almost all, as its inclusions are obvious.

We now define

$$\widetilde{T}_{k,\lambda}(u) = \widetilde{S}_{k,\lambda}(u \oplus 0), \qquad u \in \mathcal{W},$$

and consider the properties of the $\widetilde{T}_{k,\lambda}$. Evidently they are linear. If u_n is a sequence in $\mathcal{W}$ converging to u, then $u_n \oplus 0$ converges to $u \oplus 0$. As the $\widetilde{S}_{k,\lambda}$ are continuous, $\widetilde{S}_{k,\lambda}(u_n \oplus 0)$ converges to $\widetilde{S}_{k,\lambda}(u \oplus 0)$. This transcribes to the sequential continuity, hence the continuity of the $\widetilde{T}_{k,\lambda}$.

The eigenvalue result for the $\widetilde{T}_{k,\lambda}$ follows from that for the $\widetilde{S}_{k,\lambda}$ by considering elements of the form $u \oplus 0$. The completeness of the set of $\widetilde{T}_{k,\lambda}$ follows from the completeness of the $\widetilde{S}_{k,\lambda}$. For the latter property leads to

$$\widetilde{T}_{k,\lambda}(u) = 0 \qquad \Longleftrightarrow \qquad u \oplus 0 = 0,$$

and we are done. ∎

It is worth remarking that similar results hold for all self adjoint extensions of a beyond $\mathcal{H}$. Each such extension determines, besides a spectral decomposition, a complete family of generalized eigenvectors. We have considered the particular extension $a \oplus -a$ solely in order to obtain information on the product $B_\Delta B_{\Delta'}$.

5.19 Corollary Any complete family of generalized eigenvectors $\widetilde{T}_{k,\lambda}$ of a hermitian observable a determines a weak partition of unity. That is,

$$\int_\Lambda \sum_{k=1}^{d(\lambda)} \overline{\widetilde{T}_{k,\lambda}(u)}\widetilde{T}_{k,\lambda}(v)\, dm = \langle u, v \rangle, \qquad u, v \in \mathcal{W}. \tag{5.61}$$

∎

5.20 Scholium : Dirac's Formalism At this point we wish to comment on Dirac's bra and ket formalism. In his book [2], Dirac introduces two vector spaces, the space of kets, $\{ |\psi\rangle \}$, and the space of bras, $\{ \langle\psi| \}$.

The kets are supposed to determine the pure states of the system ([2], page 16). Just as we have, Dirac adopts the basic measurement principle, so these kets must be in the domain of all the observables. We have already noted that Dirac assumes the set of observables to form a non commutative algebra ([2], page 26).

Bras are asserted by him to be in one to one correspondence with kets ([2], page 20), and to be elements of the conjugate dual Hilbert space (ibid). The conjugation arises because Dirac wishes the bilinear duality pairing to coincide with the sesquilinear inner product. Thus, with our conventions,

$$\langle\psi|\varphi\rangle = \langle J(\psi), \varphi\rangle. \tag{5.62}$$

It is noteworthy that prior to asserting that bras and kets are in one-one correspondence, Dirac introduces the bras as linear functionals (ϕ on pages 18-19). The one-one correspondence then follows from the assumption that the space of wave functions is a Hilbert space, hence self dual. But as we know from the theory developed in these notes, these various conditions cannot all be satisfied by the elements of a Hilbert space. In particular, such a scheme is incompatible with the basic measurement principle.

Just as in our model, we choose the most economical extension of Dirac's ideas, and propose that : *kets are what we have called wave functions, and bras are the elements of the conjugate dual space.* With this interpretation, our model realizes Dirac's ideas in a rigorous fashion.

Perhaps it is worth emphasizing the difference between bras and kets. Every ket is a bra under the antilinear embedding map k of Chapter 4. But there are bras which are not the images of kets. These do not determine states of the system; let us call them generalized states. They determine the analogue of what are known as weights on C^*–algebras. That is, every element T determines a map τ,

$$\tau(a) = \langle T, \tilde{a}T\rangle, \qquad T \in \mathcal{W}', \tag{5.63}$$

defined on some domain in $\mathcal{L}^+(\mathcal{W})$. For generalized states, this domain is a proper subset of $\mathcal{L}^+(\mathcal{W})$.

It follows that generalized states can not be physically realized with absolute precision. We shall be able to understand this better after we discuss measurements. Before leaving this topic, let us note that some authors consider that generalized states determine relative measurements. More precisely, the ratio $\tau(a)/\tau(b)$ is interpreted as the relative mean values of a and b when measured in the generalized state T (Bogolubov et al [1]). Evidently, this ratio is defined only on the domain of τ, with due allowance made for division by zero.

Let us now relate our notation to that of Dirac. We shall employ the maps $k : \mathcal{W} \to \mathcal{W}'$, $J : \mathcal{H} \to \mathcal{H}$, and $j : \mathcal{H} \to \mathcal{W}'$ of equations (4.3), (5.11) and (5.13), respectively. We identify the space $\mathcal{K}$ of kets with the space $\mathcal{W}$ of wave functions. There will be no confusion if we simply use the ket notation of Dirac for each wave function, which we indicate as

$$|u\rangle = u. \tag{5.64}$$

Following Dirac's prescription, the space of bras is the anti-dual of the space of kets. One way of realizing this is by extending the map J from $\mathcal{H}$ to $\mathcal{W}'$. To do this, we start by recalling the dual Hermite functionals $u_n \in \mathcal{W}'$ of Lemma [4.20] :

$$[u_n, u] = \langle Jw_n, u\rangle, \qquad u \in \mathcal{W}. \tag{5.65}$$

Then

$$\widetilde{J}\left(\sum c_n u_n\right) = \sum \overline{c_n} u_n \tag{5.66}$$

is the desired conjugation map from $\mathcal{W}'$ to itself.

We now define the space of bras $\mathcal{B}$ to be the anti-linear space $\widetilde{J}\mathcal{W}'$. The elements of $\mathcal{B}$ are then

$$\langle T| = \widetilde{J}(T). \tag{5.67}$$

The duality pairing between $\mathcal{K}$ and $\mathcal{B}$ is written as an inner product, but with a solid line. Thus

$$\langle T|u\rangle = [\widetilde{J}(T), u]. \tag{5.68}$$

This is consistent with the injection of $\mathcal{W}$ into $\mathcal{W}'$.

Now we consider generalized eigenvectors in this context. In order to avoid double indices in what follows, let

$$M(\lambda) = \begin{cases} \{(1,\lambda),(2,\lambda),\ldots,(d(\lambda),\lambda)\} & \text{if } d(\lambda) \text{ is finite;} \\ \{(1,\lambda),(2,\lambda),\ldots\} & \text{otherwise} \end{cases} \tag{5.69.a}$$

and

$$\mathbb{M} = \bigcup \{ M(\lambda) : \lambda \in \Lambda \}. \tag{5.69.b}$$

By including the counting measure, we may replace the sum over $M(\lambda)$ and integral over Λ by an integral over $\mathbb{M}$ with respect to a measure we write as dm.

Let a be a hermitian observable and $(T_m : m \in \mathbb{M})$ a complete set of generalized eigenvectors for it. Dirac's notation for the bra corresponding to T_m, is

$$\langle m; a| = \widetilde{J}(T_m); \tag{5.70}$$

when the observable is clear from the context, the label a is usually omitted.

Corollary [5.19] showed that the generalized eigenvectors determined a weak partition of unity. In this notation, this would be indicated as

$$I_{\mathcal{W}} \equiv \int_{\mathbb{M}} |m; a\rangle \, \langle m; a| \, dm \qquad (\sigma(\mathcal{W}, \mathcal{W})). \tag{5.71}$$

That is, this relation is meant only in the sense of equation (5.61). Nonetheless, we must note that this notation is misleading in principle. The difficulty is that consistency of notation demands that $|m; a\rangle$ be a ket, which it is not.

The final topic concerning generalized eigenfunctions that we wish to discuss is normalization. As a first step, let a be a hermitian observable, and consider a Fourier representation obtained from a self adjoint extension as above. It is clear that $\mathcal{F}$ maps $\mathcal{W} \bigoplus \mathcal{W}$ linearly and bijectively onto $\mathcal{F}\left(\mathcal{W} \bigoplus \mathcal{W}\right)$. The same is true for

$$\mathcal{F}\mathcal{L}^{+}\left(\mathcal{W} \bigoplus \mathcal{W}\right)\mathcal{F}^{-1} = \mathcal{L}^{+}\left(\mathcal{F}\left(\mathcal{W} \bigoplus \mathcal{W}\right)\right).$$

As the graph topology from $\mathcal{L}^{+}\left(\mathcal{W} \bigoplus \mathcal{W}\right)$ is the usual topology on $\mathcal{W} \bigoplus \mathcal{W}$, we can transport the graph topology so as to make the Fourier transform a topological isomorphism. By transpose, this gives a definition of the Fourier transform of the distributions in $\mathcal{W}' \bigoplus \mathcal{W}'$. In the case of one degree of freedom and $a = p$, the momentum operator, this reduces to the usual treatment of the classical Fourier transform of tempered distributions (Trèves [1], Chapter 25).

Consider the equation

$$\beta\left(\widetilde{JX} \otimes \widetilde{Y}\right) = \langle X, Y \rangle, \qquad X, Y \in \mathcal{W} \bigoplus \mathcal{W}. \tag{5.72}$$

This defines a map $\beta \in \left(\mathcal{W}' \bigoplus \mathcal{W}'\right) \widehat{\bigotimes} \left(\mathcal{W}' \bigoplus \mathcal{W}'\right)$.

Consider this for the special case $X = u \oplus 0$ and $Y = v \oplus 0$. In the same way that one sometimes formally writes distributions as though they were functions, physicists write

$$\langle u, v \rangle = \iint_{\mathbb{M} \times \mathbb{M}} \overline{\mathcal{F}[u](m)} \, \beta_{m,n} \, \mathcal{F}[v](n) \, d(m \otimes n) \tag{5.73}$$

and

$$\beta_{m,n} = \langle m; a | n; a \rangle = \delta_{(\mathbb{M}, dm)}(m - n). \tag{5.74}$$

Whereas β is well defined, the notation of (5.73) and (5.74) is not, and even misleading, since T_m is never a ket, and an inner product on $\mathcal{W}'$ could only be defined between particular pairs of elements.

In two cases, the notation produces a familiar result. For the position operator q in one dimension, we may take $\mathcal{W}$ to be $\mathcal{S}(\mathbb{R})$, and the Fourier transform to be the identity map. As q is essentially self adjoint, the unique generalized eigenvectors are the usual Dirac delta function distributions $\{\, \delta_x : x \in \mathbb{R} \,\}$. A formal calculation gives

$$[\widetilde{J}(\delta_x), \delta_y] = \langle x|y\rangle = \delta(x-y). \tag{5.75}$$

The momentum operator p in one dimension is similar. This has a known spectral decomposition. It has a continuous spectrum $\mathbb{R}$ only, with unit multiplicity. The generalized Fourier transform is the classical Fourier transform, the spectral measure is Lebesgue measure, and the generalized eigenvectors are the exponential functions

$$E_k(x) = (2\pi)^{-1/2} \exp(-ikx), \qquad k, x \in \mathbb{R}. \tag{5.76}$$

It follows that the Fourier coefficients are just that:

$$E_k(u) = \widehat{u}_k = \widetilde{u}(k). \tag{5.77}$$

The normalization may also be directly calculated in this case, and yields

$$[\widetilde{J}(E_k), E_{k'}] = \langle k; p|k'; p\rangle = \delta(k-k'). \tag{5.78}$$

It is because of this relation that the exponential functions do not define states. However, physicists employ them as such, under the name plane waves. In classical wave theory, optics for example, these functions define states with sharp wavelengths propagating along a straight path. Even in optics such states are considered idealizations. In quantum theory, a plane wave generalized state corresponds to no information whatsoever about the position or any function of it. We shall discuss these matters further in the chapter on measurements.

In summary, then, Dirac's ideas can be rigorously justified by adopting the theory described in this monograph. His notation can be used–with extreme care. Many physicists are most at home with this notation, but we have found it to be unnecessary.

There are a number of treatments of Dirac's ideas from a rigged triple point of view. We have already made reference to Maurin's work [1-3] and the material in Gel'fand and Vilenkin [1]. A selection of other authors who have written on this topic are, eg, Antoine [1], Böhm [1], van Eijndhoven and de Graaf [1], Hermann [1], Marlow [1], Melsheimer [1] and Roberts [1-2]. ∎

6. DYNAMICS AND SYMMETRIES

6.1 THE HAMILTONIAN

Our discussion so far has concerned kinematics but not dynamics. In the algebraic formulation of quantum theory, the states refer to an instantaneous description of the system. Thus if the observable $a \in \mathcal{A}$ is measured in the state T in an ensemble of identically prepared experiments, the expected measured value is $T(a)$. Viewing this probabilistically, let us suppose that the system evolves in time under the action of all the forces present.

After a time t has elapsed, we measure the observable a again, with similar apparatus. It is possible to consider that the state T has evolved to a new state T_t during this interval, and so the new mean value is $T_t(a)$.

In particular, if T is a pure state determined by the vector $v \in \mathcal{W}$, then it is a consequence of Schrödinger's formulation of quantum mechanics that T_t is determined by the vector

$$v_t = U_t v, \qquad (t \in \mathbb{R}), \tag{6.1}$$

where $U(\mathbb{R})$ is a strongly continous unitary group, which we shall term the dynamical unitary group.

By the SNAG theorem, this group has a self adjoint generator,

$$U_t = \exp(-itH). \tag{6.2}$$

The generator H is known as the Hamiltonian operator for the system. Thus we are postulating a quantum analogue of classical Hamiltonian dynamics. Note that we are using units in which $\hbar = 1$.

For most of this chapter we shall assume that $\mathcal{W}$ is the Schwartz space $\mathcal{S}\left(\mathbb{R}^{3N}\right)$. The results we obtain will be valid for general $\mathcal{W}$ with a few obvious modifications.

It will be convenient to label the coordinates sequentially,

$$x = (x_1, \ldots, x_d),$$

using $d = 3N$ for the number of degrees of freedom. In this convention, x_3 refers to the first particle, whereas x_4 refers to the second.

A few additions are necessary to the multi-particle notation. By $q^{\mathbf{n}}$ we shall mean the operator of multiplication by $x^{\mathbf{n}}$, with $\mathbf{n} \in \mathbb{N}^d$. Similarly for the momentum operator $p^{\mathbf{n}}$. By $q^{\mathbf{n}}{}_{,j}$ we mean the multiplication operator for $\partial x^{\mathbf{n}}/\partial x_j$. For higher derivatives we write $q^{\mathbf{n}}{}_{,jk}$ in an obvious notation.

In accordance with the usual knowledge one has of a system, one starts with the kinetic energy and potential energy operators. Their sum is taken to be a candidate Hamiltonian. By some theorem similar to the Kato–Rellich theorem below, one proves that the sum is essentially self adjoint for the potential in some given class. The self adjoint extension generates a strongly continuous unitary group on the Hilbert space, as follows from the spectral calculus. We start by considering this standard situation.

The kinetic energy operator is defined on all of $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ as a domain in $L^2\left(\mathbb{R}^{3N}\right)$, by the rule

$$[K_0 v](x) = -\sum\nolimits_{j \le d} (2m_j)^{-1} \partial^2 v/\partial x_j^2. \tag{6.3}$$

We write K for the closure of K_0. We take it as known that K is self adjoint, and that $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ is a core of self adjointness for it, cf, Reed and Simon [2]. By a standard abuse of terminology, we refer to both K_0 and K as the kinetic energy.

By assumption, the forces are derivable from a potential function $\mathcal{V}$, and we write

$$[V_0 v](x) = \mathcal{V}(x) v(x), \qquad \left(v \in \mathcal{S}\left(\mathbb{R}^{3N}\right)\right). \tag{6.4}$$

6.1 Kato-Rellich Theorem The closure V of V_0 is given by the rule (6.4), but with extended domain all $v \in L^2\left(\mathbb{R}^{3N}\right)$ for which the right side is again in $L^2\left(\mathbb{R}^{3N}\right)$. Assume $\mathcal{V}$ to be real valued, measurable, and Kato bounded with respect to the kinetic energy. That is, there exist positive constants a, b, with $a < 1$, such that

$$\|Vv\| \le a\|Kv\| + b\|v\|. \tag{6.5}$$

Then

$$H = K + V \tag{6.6.a}$$

is self adjoint on the domain

$$D(H) = D(K). \tag{6.6.b}$$

$\mathcal{S}\left(\mathbb{R}^{3N}\right)$ is a core of self adjointness for H, and H restricted to it is

$$H_0 = K_0 + V_0. \tag{6.7}$$

■

Let us say that V is a Kato-Rellich class potential if it satisfies the requirements of this theorem. For such potentials, the Hamiltonian can be used to define a strongly continuous unitary group on $\mathcal{H}$, as in equation (6.2). But this is not enough for the dynamics to be compatible with the algebraic structure. For one thing, it does not guarantee that $v_t \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$ for all t, and this is a necessary and sufficient condition for the v_t to determine vector states on $\mathcal{A}$.

Hunziker [1] has found a useful sufficient condition for V in order that $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ be stable under $U(\mathbb{R})$. We present it without proof, as the proof is rather long and not especially related to algebraic methods.

6.2 Hunziker's Theorem For each $\mathbf{n} \in \mathbb{N}^d$ define the normed subspace $E_\mathbf{n}$ of $L^2\left(\mathbb{R}^d\right)$ by

$$E_\mathbf{n} = \bigcap_{|\mathbf{k}|\leq|\mathbf{n}|, r\leq|\mathbf{n}|-|\mathbf{k}|} D\left(q^\mathbf{k} H^r\right), \tag{6.8.a}$$

with norm

$$\pi_\mathbf{n}(v) = \sup_{|\mathbf{k}|\leq|\mathbf{n}|, r\leq|\mathbf{n}|-|\mathbf{k}|} \left\|q^\mathbf{k} H^r\right\|. \tag{6.8.b}$$

(a) Then $E_\mathbf{n}$ is invariant under $U(\mathbb{R})$.

(b) $U : \mathbb{R} \to \mathcal{L}\left(E_\mathbf{n}[\pi_\mathbf{n}]\right)$ is continuous, and there exists a positive constant $c_\mathbf{n}$ such that the bound

$$\pi_\mathbf{n}(v_t) \leq c_\mathbf{n}\left(1+|t|\right)^{|\mathbf{n}|} \pi_\mathbf{n}(v) \tag{6.8.c}$$

holds.

(c) For any $v \in E_\mathbf{n}$, the equation

$$q^\mathbf{n} v_t = U_t q^\mathbf{n} v + i\int_0^s U_{t-s}\left[H, q^\mathbf{n}\right] U_s v\, ds$$

holds, where the commutator is defined by

$$\left[H, q^\mathbf{n}\right] = \sum_{j\leq d}\left(-2ip_j q^\mathbf{n}{}_{,j} + q^\mathbf{n}{}_{,jj}\right).$$

The integrand is continuous in s for the $L^2\left(\mathbb{R}^d\right)$ norm, and bounded by $c_\mathbf{n}{}'\left(1+|s|\right)^{|\mathbf{n}|-1} \pi_\mathbf{n}(v)$. ∎

6.3 Corollary Let V be a real bounded $\mathcal{C}^\infty$ function with bounded derivatives of all orders. Then $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ is stable under $U(\mathbb{R})$, and $(t,v) \mapsto v_t$ is continuous from $\mathbb{R} \times \mathcal{S}\left(\mathbb{R}^{3N}\right) \to \mathcal{S}\left(\mathbb{R}^{3N}\right)$. ∎

We shall denote by Φ the class of potentials which are defined in this corollary. Note that Φ contains $\mathcal{S}\left(\mathbb{R}^{3N}\right)$.

For $V \in \Phi$, every $v \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$ satisfies the Schrödinger time dependent equation

$$i\partial v_t/\partial t = -\sum\nolimits_{j\leq d}(2m_j)^{-1}\partial^2 v_t/\partial x_j^2 + \mathcal{V}(x)v_t(x). \tag{6.9}$$

In the next section we shall consider in more detail which potentials are important for the range of phenomena our model describes.

6.2 SMOOTHED COULOMB POTENTIALS

Once again it is important to emphasize the limited range of physical phenomena we are describing, namely atomic phenomena up to medium ranges of energy and molecular phenomena up to medium molecular weights. In this range we may assume that relativistic effects need not be taken into account. The number of particles is fixed. Furthermore, we may describe any atom or molecule in terms of its constituent electrons and nucleii if we wish.

The nucleii may be treated as point particles of given mass and charge, as nuclear forces are outside our domain of study. Other complexes of particles, such as molecules, can be described as point particles for certain purposes.

This leads us to postulate that all interactions may be reduced to Coulomb interactions, at least for distances and energies which are neither too small nor too large.

The reader will probably be aware that many problems in quantum mechanics consist of finding the spectra of Hamiltonians for various non-Coulomb potentials. Although it may not be explicitly stated, these potentials are empirical and effective rather than fundamental.

The interaction potential between molecules may be determined by analyzing data from scattering experiments, cf, Bohm [1]. One striking feature of this data is that molecules tend to keep a minimal distance apart. This fact is realized by setting $\mathcal{V}(r_0) = +\infty$, where r_0 is the distance of closest approach for the molecules in question.

One must have regard for the fact that this is only an approximate extrapolation. For distances as small as r_0, the collision energies are getting towards the molecular dissociation range. This means that the experiments in question lose their validity here. At such energies the molecules break up and atomic forces take over.

Continuing to higher energies, we see that Coulomb forces eventually predominate, but only down to distances no smaller than nuclear radii. All in all, the infinite value of the potential is an idealization, and a high but finite value would do just as well.

Over the range we are describing, the data is fit best by smooth interpolation. There is no experimental indication of any non smoothness. Our conclusion is that if we wish to consider the interactions of aggregates of particles *per se*, we may describe them with a potential of class Φ. Moreover, this potential is a collective effect of the underlying Coulomb potential.

We have gone into this in detail because it is important for what follows. We define the potentials for all distances, but they are reliable only for the range our model describes. Other forces predominate outside this range, and our model is not meant to describe the resulting phenomena.

In physics terms, we may say that there are no infinitely deep wells, no infinitely high barriers, no absolutely hard walls, nor even any perfectly square wells and barriers.

We shall now prove that certain results obtained by using the class Φ potentials and those obtained by the familiar singular idealizations approach each other as the potentials do. This enables us to calculate with the well known idealizations. But for structural theorems, we must use class Φ potentials.

All this is doubly important when considering Coulomb potentials, for these are the fundamental interactions. That is, we observe experimentally that the analytic properties of all quantum mechanical properties for elementary quantum systems are derivable from the potential function

$$\mathcal{V} = \sum\nolimits_{i,j \leq N; i \neq j} v_{ij}, \tag{6.10.a}$$

where

$$v_{ij}(x_i - x_j) = e_i e_j / |x_i - x_j| \tag{6.10.b}$$

is the mutual interaction potential between particles i and j.

This potential is singular at the points of coincidence $x_i = x_j$. However, just as for molecules, to discern what the potential between charged particles ought to be at very small distances requires very high energy collisions. Such energies are outside the atomic domain. Hence the Coulomb potential determines atomic phenomena only down to small but nonzero distances. For smaller distances we wish to replace the Coulomb form by some smooth variant, such that the resulting potential is class Φ.

The justification for such a replacement is twofold. The first has been discussed: the limited energy range of our model. The second has been alluded to. We shall prove that the results obtained by the modified, smoothed and cut-off Coulomb potential approach the Coulomb results as the cut-off is removed (Dubin [2]). We note that in the proof of Proposition [6.5] just below, we have filled in some details in the corresponding proof in this reference.

The proof will show that this convergence result is true for a whole class of modifications, so the choice of modifications may be varied as convenient. This accords with the known insensitivity of scattering data to potential shape below the energy $10\,MEV$.

Our plan is to introduce the class of modified Coulomb potentials, and then to prove the convergence of the theory based on any of them to that based on the unmodified Coulomb potential. It will be reasonably clear from this that entirely similar considerations hold for square wells, hard walls, etc, and we omit the proofs for them.

6.4 Definition Let $h_n \in \mathcal{D}\left(\mathbb{R}^+\right)$ be a function such that $0 \leq h_n(x) \leq 1$ and

$$h_n(x) = \begin{cases} 1 & \text{for } x \in [0, 1/n - 1/n^2], \\ 0 & \text{for } x \in [1/n, \infty). \end{cases}$$

The h_n-cut off Coulomb function is

$$\mathcal{V}_n = \sum\nolimits_{i,j \leq N; i \neq j} v_{ij}^{(n)}, \tag{6.11.a}$$

where

$$v_{ij}(x_i - x_j)^{(n)} = [1 - h_n(|x_i - x_j|)] v_{ij}(x_i - x_j). \tag{6.11.b}$$

The cut off potential function defines a potential energy operator V_n and corresponding Hamiltonian $H_n = (K_0 + V_n)^{**}$. This Hamiltonian generates a dynamical unitary group $U^{(n)}(\mathbb{R})$.

As we shall consider only one such family $(h_n)_n$ at a time, there is no need to specify it, and so we speak simply of the cut off potentials and operators. It is also convenient to refer to the V_n as smoothed Coulomb potentials. ■

Note that the cut off Couomb potential for each pair satisfies

$$v_{ij}^{(n)} = \begin{cases} v_{ij} & \text{for } |x_i - x_j| > 1/n, \\ 0 & \text{for } |x_i - x_j| \leq 1/n - 1/n^2. \end{cases}$$

Moreover it is Φ-class, and so V_n is class Φ.

It is known that the original Coulomb potential V is Kato bounded with respect to the kinetic energy (Kato [1]), and so the domain of H is $D(K)$. As V_n is class Φ, its Kato boundedness is automatic, as observed above. Then $D(H_n) = D(K)$ as well.

The first thing that we shall prove is that $U^{(n)}$ converges strongly to U. This means that the time evolution of the pure states obtained from the cut off dynamics will approach the Coulomb evolution as the cut off is removed.

6.5 Proposition For every $f \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$ and all $t \in \mathbb{R}$, the time translations converge strongly:

$$L^2\left(\mathbb{R}^{3N}\right) - \lim_{n\to\infty} \left\| U_t^{(n)} f - U_t f \right\| = 0. \tag{6.12}$$

Proof For simplicity of notation we choose the particle masses to be $m_i = 1/2$ and the charges to be $|e_i| = 1$. These parameters can be replaced by a usual rescaling at the end, and do not in any way affect the argument.

If $g \in \mathcal{S}\left(\mathbb{R}^3\right)$, then its Fourier transform satisfies

$$[\Delta g]\tilde{}(y) = -|y|^2 \tilde{g}(y), \qquad y \in \mathbb{R}^3,$$

so

$$[(1-\Delta)g]\tilde{}(y) = \left(1 + |y|^2\right)\tilde{g}(y), \qquad y \in \mathbb{R}^3.$$

Then standard techniques for proving L^p estimates enable us to show that

$$\begin{aligned} \|g\|_\infty &\le (2\pi)^{-3/2} \|\tilde{g}\|_1 \\ &\le (2\pi)^{-1/2} \|(1-\Delta)\, g\|_2 . \end{aligned}$$

Now if $f \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$, choose a pair $1 \le i, j \le N$ with $i \neq j$, and introduce coordinates $y_1, \ldots, y_N$ with

$$y_i = x_i - x_j, \quad y_j = (x_i + x_j)/2, \quad \text{and} \quad y_k = x_k \text{ for } k \neq i, j.$$

To remind us of the change of coordinates we introduce the function $F \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$ by

$$F(y_1, \ldots, y_N) = f(x_1, \ldots, x_N).$$

By rights there ought to be an ij subscript on F, but its omission will not cause difficulties.

A rough estimate on h_n gives us the bound

$$\begin{aligned} \int_{\mathbb{R}^3} |h_n(y_i) v_{ij}(y_i)|^2 \, dy_i &= \int_0^\infty |h_n(r) v_{ij}(r)|^2 4\pi r^2 \, dr \\ &\le 4\pi e_i^2 e_j^2 \int_0^{1/n} dr \\ &= 4\pi e_i^2 e_j^2 / n. \end{aligned}$$

This enables us to obtain our first estimate of the difference between the the interparticle potentials and their cut off versions. (By $\widehat{dy_i}$ we mean that integration over y_i is to be omitted.)

$$\begin{aligned}
\left\| \left[v_{ij} - v_{ij}^{(n)} \right] f \right\|_2^2 &= \int dy_1 \dots \widehat{dy_i} \dots dy_N \left(\int |h_n(y_i) v_{ij}(y_i) F(y_1, \dots, y_N)|^2 \, dy_i \right) \\
&\leq \int dy_1 \dots \widehat{dy_i} \dots dy_N \, 4\pi e_i^2 e_j^2 / n \left(\sup_{y_i} |F(y_1, \dots, y_N)| \right)^2 \\
&\leq e_i^2 e_j^2 / n \int dy_1 \dots \widehat{dy_i} \dots dy_N \int dy_i |[(1 - \Delta_i) F] (y_1, \dots, y_N)|^2 \\
&= (e_i^2 e_j^2 / n) \, \|(1 - \Delta_i) F\|_2^2 .
\end{aligned}$$

Then

$$\left\| \left[v_{ij} - v_{ij}^{(n)} \right] f \right\|_2 \leq (e_i e_j / \sqrt{n}) (\|f\|_2 + \|\Delta_i F\|_2) .$$

We use a bound on the Fourier transform to eliminate the i dependence of the last term.

$$\begin{aligned}
\|\Delta_i F\|_2^2 &= \int |p_i|^4 \left| \tilde{F}(p_1, \dots, p_N) \right|^2 dp_1 \cdots dp_N \\
&\leq \int \left(|p_1|^2 + \cdots + |p_N|^2 \right)^2 \left| \tilde{F}(p_1, \dots, p_N) \right|^2 dp_1 \cdots dp_N \\
&= \|\Delta F\|_2^2 .
\end{aligned}$$

Recalling that all the masses have been taken to be $1/2$,

$$\left\| \left[v_{ij} - v_{ij}^{(n)} \right] f \right\|_2 \leq (2 e_i e_j / \sqrt{n}) (\|f\|_2 + \|K f\|_2) , \qquad \forall f \in D(K) .$$

Now because of the Kato boundedness of the Coulomb potential, there exists a constant $c > 0$ such that

$$\|K f\|_2 \leq 2 \|H f\|_2 + 2c \|f\|_2 , \qquad \forall f \in D(K) .$$

Thus

$$\left\| \left[v_{ij} - v_{ij}^{(n)} \right] f \right\|_2 \leq (4 e_i e_j / \sqrt{n}) (\|H f\|_2 + (c+1) \|f\|_2) , \qquad \forall f \in D(K) .$$

Now we note that if $f \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$, then $U_s f \in D(K)$ for all $s > 0$. Note also that U_s commutes with H, and so we have

$$\left\| \left[v_{ij} - v_{ij}^{(n)} \right] U_s f \right\|_2 \leq (4 e_i e_j / \sqrt{n}) (\|H f\|_2 + (c+1) \|f\|_2) , \qquad \forall f \in \mathcal{S}\left(\mathbb{R}^{3N}\right) .$$

As in Cook's method in scattering theory, Reed and Simon [3], we have the inequality

$$\begin{aligned}\left\|U_t f - U_t^{(n)} f\right\| &= \left\|U_{-t}^{(n)} U_t f - f\right\| \\ &\leq \int_0^t \left\|U_s^{(n)} [V - V_n]\, U_s f\right\| ds \\ &\leq \sum\nolimits_{i,j\leq N; i\neq j} \int_0^t \left\|[v_{ij} - v_{ij}^{(n)}] U_s f\right\| ds.\end{aligned}$$

We can now sum over pairs of indices. Using the difference inequality we have just shown, and remembering that $e_i = \pm 1$, we get

$$\left\|U_t f - U_t^{(n)} f\right\| \leq 2tN(N-1)n^{-1/2} \left(\|Hf\|_2 + (c+1)\|f\|_2\right).$$

The limit $n \to \infty$ now proves the assertion, and we are done. ■

6.6 Corollary Let $\mathcal{B}$ be a generalized spectral family under which $\mathcal{W}$ is stable. Then for all $f \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$, all times t and all Borel sets Δ,

$$\lim\nolimits_{n\to\infty} \langle U_t^{(n)} f, \mathcal{B}_\Delta U_t^{(n)} f\rangle = \langle U_t f, \mathcal{B}_\Delta U_t f\rangle. \tag{6.13}$$

■

This is an easy application of the Cauchy-Schwarz inequality, and we omit it.

6.7 Remarks It is the content of these last two results which constitutes the convergence of the H and H_n theories as $n \to \infty$. Note that it is not true that the time evolved states converge. But this must be expected, as $U_t f$ is not an element of $\mathcal{W}$ in general. Thus Proposition [6.5] is the best that could be expected.

Corollary [6.6], in contrast, shows that the expectation values of the theories do converge. In view of the nature of quantum measurement theory, this is an effective substitute for the convergence of states. ■

These convergence results imply the convergence of the spectra of the Hamiltonians in the following sense.

6.8 Proposition In the generalized strong sense of Kato [1],

$$H_n \to H. \tag{6.14}$$

The resolvents converge in the generalized strong sense for $\mathrm{Im}(z) \neq 0$:

$$R_n(z) \to R(z). \tag{6.15}$$

Hence every open subset of $\mathbb{R}$ containing a point of the spectrum of H contains at least one point of the spectrum of H_n for n sufficiently large. The corresponding spectral projections converge in the strong sense:

$$L^2\left(\mathbb{R}^d\right) - \lim_{t_n \to t} P_n(t_n) = P(t).$$

For the case of two particles, consider their relative motion. The eigenvalues of H are $-1/n^2$, where n is now the principal quantum number,and $n \geq 1$. To each n there corresponds n eigenvalues of H_p, written

$$E^{(p)}(1,n), \ldots, E^{(p)}(n,n),$$

all in the neighbourhood of $-1/n^2$.

Thus the n^2–fold degeneracy of $-1/n^2$ is partially broken. Due to rotational symmetry, each $E^{(p)}(j,n)$ is n-fold degenerate. As $p \to \infty$,

$$E^{(p)}(j,n) \to -1/n^2, \qquad 1 \leq j \leq n.$$

Proof Our estimates for $s = 0$ imply that

$$\|(H_n - H)f\| \to 0$$

for all $f \in \mathcal{S}\left(\mathbb{R}^{3N}\right)$. As $\mathcal{S}\left(\mathbb{R}^{3N}\right)$ is a core for both H and H_n, the first part follows from Kato [1], VIII.1, Cor 1.6. The second part follows from VIII.2, theorem 1.14, ibid.

For two particle relative motion, the spectrum of H below zero consists only of isolated eigenvalues of finite multiplicity. Moreover, the forms associated with the H_p increase to the form for H. The result now follows from Kato [1], VIII.4, Theorem 3.15. ■

We have not analyzed the stability of the isolated eigenvalues for $N \geq 3$.

Hereafter we shall assume that all potentials are of class Φ, and the Coulomb potential is smoothed as above.

6.3 DYNAMICAL AUTOMORPHISMS

In the previous section we stated our belief that the fundamental forces relevant to the systems under consideration are the smoothed Coulomb potentials. This should be kept in mind, but for the remainder of this section it is only necessary that the potential V be of class Φ.

The dynamical group $U(\mathbb{R})$ determines the evolution of vector states through equation (6.1). Since every state is a sum of vector states, equation (6.1) generalizes to all of $\mathcal{A}'$, as we shall show. By transposition it then determines an automorphism group of $\mathcal{A}'$.

Suppose an observable a is measured in a state T at time zero. One may envision an ensemble of identically prepared experiments. The mean, or expected value is

$$\mathrm{EXP}\,(T; a; 0) = T(a).$$

Now let a time interval t pass and redo the experiment, obtaining an expected value $\mathrm{EXP}\,(T; a; t)$. There are two equivalent ways of computing this new value. We may consider that the state has remained the same and the observables have evolved. Conversely, we may consider that the observables have remained the same and the state has evolved.

The first point of view is known as the Heisenberg picture, and the second as the Schrödinger picture. The distinction between them is analogous to the active and passive views of actions of transformation groups on sets.

It is important to note that we are working in the locally convex algebra setting. This means that we must prove continuity and differentiability with respect to the relevant topologies. It is not enough, for instance, to consider the strong continuity of the dynamical unitary group on Hilbert space. Thus we must apply the theory of semigroups on locally convex spaces. The difficult part of the next result is to prove that the algebra and state dynamics are given by locally equicontinuous groups of type C_0.

6.9 Proposition (a) We can define a locally equicontinuous type C_0 one parameter group

$$\tau : \mathbb{R} \to \mathcal{L}(\mathcal{A})$$

by setting

$$\tau_t(a) = U_{-t} a U_t, \qquad t \in \mathbb{R},\ a \in \mathcal{A}. \tag{6.16}$$

This group has an infinitesimal generator which is an element of $\mathcal{L}(\mathcal{A})$, and by differentiation we obtain the Heisenberg equations of motion:

$$d\tau_t(a)/dt = i\,[H, \tau_t(a)]\,. \tag{6.17}$$

(b) We can also define a locally equicontinuous type C_0 one parameter group

$$\tau' : \mathbb{R} \to \mathcal{L}(\mathcal{A}')$$

by setting

$$\tau_t'(\rho) = U_t \rho U_{-t}, \qquad t \in \mathbb{R},\ \rho \in \mathcal{A}'. \tag{6.18}$$

This group has an infinitesimal generator which is an element of $\mathcal{L}(\mathcal{A}')$, and by differentiation we obtain the Schrödinger equations of motion:

$$d\rho_t/dt = -i\,[H, \rho_t]\,, \tag{6.19}$$

where we use the obvious abbreviation ρ_t for $\tau_t'\rho$.

The triple

$$[\![\mathcal{A}, \mathrm{S}, \tau\,(\mathbb{R})]\!] \tag{6.20}$$

is known as the Heisenberg picture, and the triple

$$[\![\mathcal{A}, \mathrm{S}, \tau'\,(\mathbb{R})]\!] \tag{6.21}$$

is known as the Schrödinger picture. These two pictures are physically equivalent, since

$$[\tau_t' T]\,(a) = T\,[\tau_t a] \tag{6.22}$$

for all $T \in \mathcal{A}'$, $a \in \mathcal{A}$, and $t \in \mathbb{R}$.

Proof The results of Hunzicker's theorem show that the dynamical group

$$U : \mathbb{R} \to \mathcal{L}\,(\mathcal{W})$$

is a locally equicontinuous type C_0 one parameter group, with infinitesimal generator $-iH$. We have

$$U_t x - x = -i \int_0^t U_s H x\, ds, \qquad t \in \mathbb{R},\ x \in \mathcal{W},$$

and

$$\pi_{\mathbf{n}}(U_t x) \le c_{\mathbf{n}}(1 + |t|)^{|\mathbf{n}|}\, \pi_{\mathbf{n}}(x), \qquad \mathbf{n} \in \mathbb{N}^d,\ t \in \mathbb{R},\ x \in \mathcal{W}.$$

It is clear that $\tau : \mathbb{R} \to \mathcal{L}\,(\mathcal{W})$ is a one parameter group. If B is a bounded subset of $\mathcal{W}$, then so is

$$C = \bigcup_{|t| \le 1} U_t\,(B \cup HB)\,.$$

With this notation, let $|t| \le 1$. Then

$$\langle x, (\tau_t - 1)ax\rangle = -i \int_0^t \left[\langle U_t x, a U_s H x\rangle - \langle U_s H x, ax\rangle\right]\, ds,$$

from which it follows that

$$p_B([\tau_t - 1]a) \le 2|t| p_{C,C}(a).$$

It is immediate that τ is of type C_0.

Next, consider

$$\begin{aligned} p_B(\tau_t a) &\le \sup_{x \in B} |\langle U_t x, a U_t x\rangle| \\ &\le p_C(a). \end{aligned}$$

This is the definition of local equicontinuity for τ.

By a similar approach, but somewhat longer and not very instructive, we can show that

$$\lim_{t \to 0} (\tau_t a - a)/t = i[H, a]$$

in $\mathcal{A}$. Thus τ has an everywhere defined infinitesimal generator, given by the commutator action

$$\mathcal{G} : a \mapsto [H, a], \qquad a \in \mathcal{A}.$$

(b) Define $\tau' : \mathbb{R} \to \mathcal{L}(\mathcal{A}')$ by setting τ'_t to be the transpose of τ_t. Clearly τ' is a one parameter group. Since $\{\tau_t : |t| \le 1\}$ is equicontinuous, so is $\{\tau'_t : |t| \le 1\}$.

If $\xi \in \mathcal{A}'$, choose a bounded subset B of $\mathcal{W}$ satisfying

$$|[\xi, a]| \le p_B(a), \qquad a \in \mathcal{A},$$

and define the set C from B as above. For $|t| \le 1$,

$$|[\tau'_t \xi - \xi, a]| \le p_B(\tau_t a - a) \le 2|t| p_{C,C}(a).$$

It follows that for any bounded subset D of $\mathcal{A}$,

$$p_D(\tau'_t \xi - \xi) \le 2|t| \sup_{a \in D} p_{C,C}(a), \qquad |t| \le 1.$$

Hence $\tau' : \mathbb{R} \to \mathcal{L}(\mathcal{A}')$ is of type C_0. The known isomorphism between $\mathcal{A}'$ and T clearly yields the given representation of τ' acting on density matrices.

A close investigation of the proof of the existence of the infinitesimal generator of τ shows the following. For every bounded subset B of $\mathcal{W}$ there exists a bounded subset C of $\mathcal{W}$ and a certain function $f : \mathbb{R} \to [0, \infty)$, which does not depend on B, such that

$$p_B(i[H, a] - (\tau_t a - a)/t) \le f(t) p_{C,C}(a).$$

Combining this with transposition, it is easy to show that the group τ' has an everywhere defined infinitesimal generator, equal to the transpose of $\mathcal{G}$. The Schrödinger equation is now immediate. That τ'_t preserves density matrices follows from the fact that τ_t is an algebra automorphism. Finally, equation (6.22) is obvious. ■

We wish to end this section with the following result due to Ehrenfest [1]. Its proof is a simple computation and is omitted.

6.10 Ehrenfest's Theorem Newton's equations of motion hold for expected values. That is,

$$d/dt\,[\tau_t\,(p_j)] = -\tau_t\,[\partial V/\partial x_j] \tag{6.23.a}$$

and so

$$d/dt\,[\tau_t' T]\,(p_j) = -\,[\tau_t' T]\,(\partial V/\partial x_j)\,. \tag{6.23.b}$$

■

Note carefully that this result does not imply a simple limit relation between quantum and classical mechanics. This is because

$$\partial V/\partial x_j\,[T(x)] \neq T\,[\partial V/\partial x_j(x)]\,.$$

The sense in which the quantum evolution fluctuates around the classical path for small $\hbar$ may be found in Thirring [1], 3.3.13.

6.4 TIME INVARIANT STATES

In this section we shall assume that the system dynamics is determined by a Hamiltonian H for which V is class Φ. We shall assume that H has eigenvalues $\{E_1, E_2, \ldots\}$ in $\mathcal{W}$. This set may contain all or only some of the eigenvalues of H; it might even be empty. Let us write $\{e_1, e_2, \ldots\}$ for the associated orthonormal eigenvectors. We do not assume that the eigenvectors form a basis for the system Hilbert space.

Consider an electron in orbit around a proton in the Bohr theory. The state of the electron is characterized by the fact that its energy is definite and unvarying in time. Other variables, such as the position and momentum of the electron take definite values at all times (Bohr [1]).

In wave mechanics this semiclassical picture does not persist. There are vectors of definite energy for a given Hamiltonian, and this energy is fixed in time. But other observables, such as position and momentum, do not take definite values in such states. The pure states corresponding to such vectors are known as stationary states, or time invariant states.

For a stationary pure state, the mean value of any observable is independent of time. In particular, if the probability of finding a particle outside a compact region is small at one time, it remains small for all times. In this sense, such states correspond to classical orbits which remain in compact regions. Thus stationary states are also known as bound states.

Bound states are more precisely defined as corresponding to the poles of the S-matrix, and one then proves that these states are stationary. We shall not consider scattering theory here, and refer the reader to the literature: Putnam [1], Reed and Simon [2], Thirring [1].

Consider a state which is a convex combination of pure stationary states. It, too, is stationary, and the mean value of any hermitian observable a as a function of time,

$$\tau_t'(T)(a) = \sum\nolimits_{j,k} r_j r_k \langle e_j, a e_k\rangle \exp[-it(E_j - E_k)],$$

is an almost periodic function. Consequently, its ergodic mean average exists, but the limit $t \to \infty$ does not, in general.

Then if the probability of finding a particle outside a compact region is small at one time, it is small for all times, although it may oscillate rapidly. Such states are also bound, just as the pure stationary states are. The old quantum theory, prior to Heisenberg's work, dealt only with such states. This is because they support an approximate notion of particle orbit.

We know that the spectrum of the Hamiltonian consists of a continuous as well as a discrete part, in general. The continuous part is associated with scattering, and corresponds to at least partial ionization or dissociation.

For such scattering states, the positive energy is inconsistent with time invariance. Consider the scattering of electrons by central forces at intermediate energies as an example. The last thing one would expect would be an unchanging expectation for finding the electrons confined to a given fixed spatial region. But for a stationary state, this is precisely what would occur. Fortunately for the compatibility of the physics and the mathematics, we are able to show that there are no stationary states associated with the continuous spectrum. Note that we have adopted the convention of considering a state as stationary if its relative part is; we always hive off the centre of mass contribution.

The next proposition asserts this, namely that stationary states are necessarily convex combinations of pure stationary states. The proof rests on a result which is true for more general symmetries of the system. As it is no more difficult to prove the general result, we shall do so in Proposition [6.32].

6.11 Proposition A functional $T \in \mathcal{A}'$ is said to be stationary, or time invariant, if

$$\tau_t'(T) = T, \qquad (t \in \mathbb{R}). \tag{6.24}$$

The time translations are with respect to the relative Hamiltonian, if that is relevant.

The set of stationary states is convex; its extreme points are said to be ergodic with respect to $\tau'(\mathbb{R})$. Then every ergodic state is pure.

A vector state

$$T(a) = \langle u, au \rangle$$

is ergodic if and only if $u \in \mathcal{W}$ is an eigenvector if the Hamiltonian H.

A general stationary functional T may be reduced into ergodic components:

$$T(a) = \sum r_n T_n(a),$$

where each

$$T_n(a) = \langle v_n, a v_n \rangle,$$

is stationary.

Proof Only the proof that a stationary pure state is an eigenstate will be given here. The remainder will follow from the general theory to be proved in Proposition [6.32]. Let T be a stationary state determined by the unit vector $u \in \mathcal{W}$. Let $P_v \in \mathcal{A}$ denote the projection onto $v \in \mathcal{W}$. For any real t, the function

$$F_t(v) = |\langle U_t u, v \rangle|^2, \qquad v \in \mathcal{H},$$

is continuous from $\mathcal{H}$ to $\mathbb{R}$. Stationarity implies that

$$F_t(v) = \tau_t' T(P_v) = T(P_v) = F_0(v)$$

for all $v \in \mathcal{W}$. Then

$$\{ v \in \mathcal{H} : F_t(v) = F_0(v) \}$$

is a closed subset containing the dense set $\mathcal{W}$. Consequently it must be $\mathcal{H}$ itself. Hence $F_t = F_0$ for all t on all of $\mathcal{H}$.

It follows that the orthogonal complements of the $\{ U_t u \}$ are all identical, and so $U_t u$ belongs to the linear span of $\{ u \}$.

Combining this with the group law, we see that

$$U_t u = k(t) u,$$

where k is a continuous character on $\mathbb{R}$. We can therefore write

$$k(t) = e^{-iEt}$$

for some real number E. Differentiation now yields

$$Hu = Eu,$$

completing the first part of the proof. ∎

We are now in a position to state the axiom for time translations.

Axiom 5. The energy observable for the system is the Hamiltonian operator H, equation (6.6.a). For atomic and molecular systems, the fundamental potential is the underlying Coulomb potential. Considering distances and energies appropriate to such systems, a smoothed Coulomb potential such as equation (6.11.b) may be used. For the limited description of certain phenomena, appropriate empirical potentials may be used, such as wells and barriers. These must be such that $\mathcal{W}$ is stable under the dynamical unitary group

$$U_t = \exp(-itH/h).$$

A sufficient condition for this is that $V \in \Phi$. The dynamical group determines the continuous automorphism groups $\tau(\mathbb{R})$ and $\tau'(\mathbb{R})$ for $\mathcal{A}$ and $\mathcal{A}'$, respectively. The viewpoint wherein the observables remain fixed in time and the states evolve, is known as the Schrödinger picture, $[\![\mathcal{A}, \mathrm{S}, \tau'(\mathbb{R})]\!]$. The equation of motion in this picture is the generalized Schrödinger equation, equation (6.19). An equivalent viewpoint is the Heisenberg picture, $[\![\mathcal{A}, \mathrm{S}, \tau(\mathbb{R})]\!]$, wherein the states remain fixed, and the observables evolve in time. The equation of motion in this picture is equation (6.17). This subsumes Newton's equations as expectation values. If spin and statistics are included, the potential must be symmetrized. ■

Questions concerning the spectrum of the Hamiltonian are not intrinsically algebraic. Discussions may be found in a variety of texts, eg, Kato [1], Kemble [1], Putnam [1], Reed and Simon [1–3], Thirring [1]. The following examples are given solely in order to emphasize various points touched at in the previous work.

6.12 Free Evolution The potential $V = 0$ is certainly of class Φ. The Hamiltonian is the kinetic energy alone, $H = K$, and its spectrum consists entirely of an absolutely continuous component,

$$\sigma(K) = \sigma_{ac}(K) = \mathbb{R}_+. \tag{6.25}$$

There are no eigenvectors, showing that $V \in \Phi$ is insufficient for the existence of stationary states. The smooth functions

$$E_p(x) = \exp(-ip \cdot x), \qquad (p \in \mathbb{R}^d), \tag{6.26.a}$$

are distributions, $E_p \in S'(\mathbb{R}^d)$, satisfying

$$K\,E_p = \sum\nolimits_j (p_j^2/2m_j)E_p \tag{6.26.b}$$

$$= \varepsilon(p)\,E_p. \tag{6.26.c}$$

Hence the E_p are generalized eigenvectors (Gel'fand and Vilenkin [1]) for K.

Let us relate this example to to the spectral theory notation of §5.6. Let $\Lambda = \mathbb{R}$ and $d(\lambda) = 2$ for all λ, as the spectrum of K is everywhere two-fold degenerate. For convenience we shall consider one degree of freedom and let $k \in \{-1, +1\}$. Let $\widetilde{\mathcal{H}}_{\pm,\lambda}$ be the one dimensional space spanned by $E_{\pm\lambda}$, and so

$$\widetilde{\mathcal{H}}_{\lambda} = \widetilde{\mathcal{H}}_{-,\lambda} \bigoplus \widetilde{\mathcal{H}}_{+,\lambda}.$$

Choose $d\mu(\lambda)$ to be Lebesgue measure on the line, the spectral function $F(\lambda)$ to be $\lambda^2/2m$. These choices determine a spectral decomposition in the sense of §5.6.

Let us reserve the tilde for the classical Fourier transform, and $\mathcal{F}$ for the spectral transform. Then for any $v \in \mathcal{S}(R)$,

$$\mathcal{F}(v) = \int_{\mathcal{R}_+}^{\oplus} [\tilde{v}(-\lambda) \oplus \tilde{v}(+\lambda)]\, d\lambda,$$

with

$$\tilde{v}(\pm\lambda) = E_{\pm\lambda}(v) = \langle \mp, \lambda | v \rangle.$$

The weak partition of unity is given by

$$\begin{aligned}
\langle v, \left\{ \int_{\mathcal{R}_+}^{\oplus} \bigoplus_{k=-1}^{+1} |k,\lambda\rangle\langle k,\lambda|\, d\lambda \right\} u \rangle &= \int_0^{\infty} \sum_{k=-1}^{+1} \tilde{v}(k\lambda)^* \tilde{u}(k\lambda)\, d\lambda \\
&= \int_{\mathbb{R}} \tilde{v}(p)^* \tilde{u}(p)\, dp \\
&= \langle v, u \rangle, \qquad u, v \in \mathcal{S}(R).
\end{aligned}$$

Normalization is given by the formal expression

$$\langle k, \lambda | k', \lambda' \rangle = \delta\,(k\lambda - k'\lambda'),$$

whose meaning was examined in §5.6.

The generalized state $T_{k,\lambda}$ determined by $\langle k, \lambda|$ has none of the basic observables in its domain. It may be approximated by sequences of vector states, eg,

$$v_n = \sum_{j=0}^{n} i^j w_j(k\lambda) w_j.$$

The dynamical unitary group can be given explicitly, namely

$$[U_t v](x) = (m/2\pi i t)^{d/2} \int \exp\left(im|x-y|^2/2t\right) v(y)\, dy. \qquad (6.26.d)$$

It is seen that U has a continuous kernel. ■

6.13 A Hyperbolic Well For one degree of freedom, consider the potential function

$$\mathcal{V}(x) = -V_0/\cosh^2(x/a). \tag{6.27}$$

This is a Φ class potential, and the spectral properties of H can be found explicitly, Goldman et al [1].

The spectrum is

$$\sigma(H) = \sigma_d(H) \bigcup \sigma_{ac}(H) \tag{6.28.a}$$

with

$$\sigma_{ac}(H) = \mathbb{R}_+ \tag{6.28.b}$$

and

$$\sigma_d(H) = \left\{ E_n = -\varepsilon\,[\beta - (2n+1)]^2 : n = 0, 1, \ldots, N \right\}. \tag{6.28.c}$$

The energy constants are

$$\varepsilon = 1/2ma^2 \qquad \text{and} \qquad \beta = \sqrt{1 + 4V_0/\varepsilon}.$$

The eigenvalues are negative, and the greatest is determined by the greatest integer N which is less than $(\beta - 3)/2$.

The eigenvalues are multiplicity free. Corresponding to the eigenvalue E_n is the eigenfunction

$$v_n(x) = A_n \cosh^{-(\beta-1)/2}(x/a) V_n(x),$$

where

$$V_n(x) = \begin{cases} {}_2F_1\left(-k, k - (\beta - 1)/2, 1/2; -\sinh^2(x/a)\right) & \text{for } n = 2k; \\ \sinh(x/a)\,{}_2F_1\left(-k, k - (\beta - 3)/2, 3/2; -\sinh^2(x/a)\right) & \text{for } n = 2k+1. \end{cases}$$

The constant A_n is chosen so that v_n is normalized.

These eigenfunctions are evidently in $\mathcal{W}$, but do not form a basis for $L^2\left(\mathbb{R}^1\right)$. The point 0 is in the continuous spectrum in general. If and only if the constants are such that 0 is the highest eigenvalue, there is an eigenvalue in the continuum. In this case, note, it is isolated from the other eigenvalues, and not an accumulation point of the discrete spectrum.This example is typical of the smooth one dimensional wells encountered in Physics. As far as the authors know, it is an open problem to find conditions on V such that (1): the space $\mathcal{W}$ is stable under the dynamical unitary group and (2): the eigenfunctions of H are elements of $\mathcal{W}$, even in one dimension.

There are results concerning the properties of eigenfunctions, but they are not directly relevant to this problem. For $V \in \Phi$, it is easy to prove that if an eigenfunction v (1) is $\mathcal{C}^2$, and (2) if both $x^r v$ and $x^r v'$ are bounded for all $r \in \mathbb{N}$, then $v \in \mathcal{S}(\mathbb{R})$. If only the first condition is satisfied, $v \in \mathcal{C}^\infty$.

6.14 The Hydrogen Atom The first success of Schrödinger's wave mechanics was the complete solution for the Hydrogen atom. We shall not solve this problem here, as it is solved in almost all texts on quantum mechanics. We wish to point out some salient features of the solution, though.

The original two particle Hilbert space $\mathcal{H}$ can be written as $\mathcal{H}_{CM} \otimes \mathcal{H}_{REL}$ after the unitary transformation to centre of mass and relative coordinates. The wave function space is similarly factored by this transformation.

The transformation allows the Hamiltonian to be written as

$$H = H_{CM} + H_{REL}, \tag{6.29.a}$$

where

$$H_{CM} = -(1/2M)\nabla^2_{CM} \tag{6.29.b}$$

and

$$H_{REL} = -(1/2m)\nabla^2_{REL} - Ze^2/(x \cdot x)^{1/2} \tag{6.29.c}$$

in an obvious notation.

Because H_{CM} is the free Hamiltonian, it has no eigenvectors. It follows that if we are being precise in our language, the hydrogen atom has no stationary states. In contrast, the relative Hamiltonian does have eigenvectors, and they are all elements of $\mathcal{S}\left(\mathbb{R}^3\right)$. This example serves to show that the condition $V \in \Phi$ is not necessary for stationary states of the algebra to exist.

Consider the vector states of the atom determined by vectors of the form $u_{CM} \otimes v_{REL}$. Suppose v_{REL} is an eigenvector of H_{REL}. Such states are stationary for the relative subalgebra. That is, the algebra generated by observables of the form $I_{CM} \otimes a_{REL}$. This is what physicists mean by stationary states of the atom.

The discrete spectrum of H_{REL} and its eigenvectors may be found by introducing spherical polar coordinates in Schrödinger's equation. The equation then separates into three Sturm Liouville equations. These can be solved by power series methods. The square integrability leads to the eigenvalues in familiar fashion.

A more interesting solution is obtained by utilizing the Lenz-Runge operator, which commutes with the Hamiltonian. Certain combinations of this and the angular momentum constitute a representation of $so(4,1)$. Simple raising and lowering operator methods then determine the eigenfunctions, cf, Thirring [1].

The discrete spectrum of H_{REL} turns out to be

$$\sigma_d(H_{REL}) = \left\{ -\varepsilon/n^2 : n = 1, 2, \dots \right\}, \tag{6.29.d}$$

with ε, the ionisation energy, equal to 13.6 electron volts.

The nth eigenvalue has multiplicity n^2, or as physicists say, is n^2-fold degenerate. The standard eigenvectors for E_n are, in polar coordinates,

$$v_{nlm}(r, \theta, \varphi) = N_{nlm}\, R_{nl}(r)\, Y_{lm}(\theta, \varphi). \tag{6.30.a}$$

Y_{lm} are the usual spherical harmonics; the indices l and m refer to the eigenvalues of the square and third component of angular momentum. We have encountered these functions previously, in Section 2.8 :

$$L \cdot L\, v_{nlm} = l(l+1) v_{nlm}, \tag{6.30.b}$$

and

$$L_3\, v_{nlm} = m\, v_{nlm}. \tag{6.30.c}$$

The ranges of the eigenvalues are

$$l = 0, 1, \ldots, n-1 \quad \text{and} \quad m = -l, -l+1, \ldots, l-1, l.$$

The radial eigenfunctions are generalized Laguerre polynomials modulating an exponential damping factor. Explicitly, $n = 1, 2, \ldots$, and

$$R_{nl}(r) = \left(\frac{2rZ}{na_0}\right)^l e^{-rZ/na_0}\, L_{n+l}^{2l+1}\left(\frac{2rZ}{na_0}\right). \tag{6.30.d}$$

The constant N_{nlm} is for normalization:

$$N_{nlm} = \left[\left(\frac{2Z}{na_0}\right)^3 \left(\frac{2l+1}{4\pi}\right) \frac{(l-|m|)!(n-l-1)!}{2n(l+|m|)![(n+l)!]^3}\right]^{1/2} \tag{6.30.e}$$

Thus $\|v_{nlm}\| = 1$. Here $a_0 = \hbar^2/me^2$ is the Bohr radius, $.529 \times 10^{-8}$ *cm.*

By analytic continuation, the functions v_{nlm} can be continued from negative to positive energy. These continuations are distributions, and may be called continuum wavefunctions. This corresponds to the result

$$\sigma_{ess}(H_{REL}) = \mathbb{R}^+, \tag{6.31.a}$$

$$\sigma_{sing}(H_{REL}) = \emptyset. \tag{6.31.b}$$

The point 0 is an accumulation point of the spectrum, as can be seen by the formula for E_n. There are no eigenvalues in the continuum, cf, Kemble [1].

The eigenfunctions form an orthonormal basis for the Hilbert subspace associated with the discrete spectrum. Together with the continuum distributions they comprise an expansion family for all of $L^2(\mathbb{R}^3)$.

In this regard it is natural to ask why the eigenfunctions alone do not constitute a basis for $L^2(\mathbb{R}^3)$. Of course they cannot on general principles, as the discrete spectrum is upper and lower bounded. But on the other hand, Sturm Liouville eigenfunctions are complete, cf, Courant and Hilbert [1]. The conflict is removed by noting that the simple scaling of the radial variable r to the Sturm Liouville variable depends on the eigenvalue: $r \to 2rZ/na_0$, cf, Kemble [1].

Regarding $\mathcal{S}(\mathbb{R}^3)$ we wish to note the following. For any $f \in \mathcal{S}(\mathbb{R}^3)$, define the function

$$f_{lm}(r) = \int_{S^2} f\,\overline{H_{lm}}, \tag{6.32.a}$$

where the integral is with respect to to the Haar measure over the sphere, and we have introduced the harmonic polynomials

$$H_{lm} = r^{-l} Y_{lm}. \tag{6.32.b}$$

Then $f_{lm} \in \mathcal{S}(\mathbb{R}^+)$, and the expansion

$$f(x) = \sum_{m=-\infty}^{+\infty} \sum_{l=|m|}^{+\infty} f_{lm}(r) H_{lm}(x) \tag{6.32.c}$$

converges in $\mathcal{S}(\mathbb{R}^3)$. For a proof of this valid in d dimensions, and a dual expansion for tempered distributions, see Tröger [1]. This supplements equation (2.66) . For a discussion of the spectrum of multiparticle atoms, see Thirring [1].

6.5 AUTOMORPHISMS AND SYMMETRIES

The dynamical group action $U(\mathbb{R})$ of the previous sections is but one example of transformations under which the algebra is stable. They are known as automorphisms. Of particular interest are families of automorphisms which constitute a representation of a group. $\tau(\mathbb{R})$ is an example. The formal definitions are these.

6.15 Definition (a) Let $\mathcal{A}$ be a unital topological *-algebra ordered by a positive cone $\mathcal{K}$. By an automorphism of $\mathcal{A}$ we mean a linear transformation $\alpha : \mathcal{A} \to \mathcal{A}$ for which

$$\alpha(ab) = \alpha(a)\alpha(b) \tag{6.33.a}$$

and

$$\alpha(a)^* = \alpha(a^*) \tag{6.33.b}$$

for all a, $b \in \mathcal{A}$.

The automorphism α is said to be positive if $\mathcal{K}$ is stable under it. It is said to be continuous if it belongs to $\mathcal{L}(\mathcal{A})$.

We write $\mathrm{Aut}(\mathcal{A})$ for the set of automorphisms. We indicate positivity by a subscript $+$, and continuity by a subscript c.

(b) A group G is said to be represented as automorphisms if there exists a group homomorphism

$$\alpha : G \to \mathrm{Aut}(\mathcal{A}).$$

Let G be a topological group, and suppose that each α_g is continuous. Then $\alpha(G)$ is said to be continuous if the function $g \to \alpha_g$ is strongly continuous.

(c) A functional $T \in \mathcal{A}'$ is said to be invariant under the automorphism α if $T \circ \alpha = T$. It is invariant under $\alpha(G)$ if $T \circ \alpha_g = T$ for all $g \in G$. If it is clear which automorphism group is meant, we say that T is G-invariant.

The set of G-invariant states is convex and *-symmetric. An extreme point of this set is known as a G-ergodic state.

(d) A continuous automorphism α of $\mathcal{L}^+(\mathcal{W})$ is said to be unitarily implemented if there exists a map $U \in \mathcal{L}^+(\mathcal{W})$ which extends to a unitary operator on $\mathcal{H}$ such that

$$\alpha(a) = UaU^+. \tag{6.34.a}$$

For a continuous group $\alpha(G)$ of automorphisms, this is varied to the existence of a strongly continuous map $U : G \to \mathcal{L}(\mathcal{W})$ which extends to a strongly continuous unitary group on $\mathcal{H}$, with

$$\alpha_g(a) = U_g a U_{g^{-1}}. \tag{6.34.b}$$

Notice that all such automorphisms are inner, meaning that each U or U_g is an element of $\mathcal{L}^+(\mathcal{W})$. ■

It is tedious continually to distinguish single automorphisms from groups of them. We will avoid this by considering single automorphisms to represent the one element group.

An analysis of our proof of the continuity of the time translation automorphism group $\tau(\mathbb{R})$ reveals a pattern that can be considerably generalized.

6.16 Proposition Let G be a metrisable Hausdorff topological group, and let $U : G \to \mathcal{L}(\mathcal{W})$ be a strongly continuous group homomorphism which extends to a strongly continuous unitary group on $\mathcal{H}$. Then $\alpha : G \to \mathrm{Aut}(\mathcal{L}^+(\mathcal{W}))$, defined by equation (6.34.b), is a continuous automorphism group.

Proof Let us, for the while, ignore spin and statistics for simplicity. Then $\mathcal{W} = s^{(d)}$ for some d. We know that $\mathcal{W}$ has a basis $\{ e_{\mathbf{n}} \}$, and that for any bounded subset B of $\mathcal{W}$ we can find a $v = \sum v_{\mathbf{n}} e_{\mathbf{n}}$ in $\mathcal{W}$ with $v_{\mathbf{n}} \geq 0$ for all $\mathbf{n}$, such that

$$B \subseteq B_v = \left\{ \sum z_{\mathbf{n}} v_{\mathbf{n}} e_{\mathbf{n}} : |z_{\mathbf{n}}| \leq 1 \right\}, \quad .$$

with B_v bounded.

Let $U : G \to \mathcal{L}(\mathcal{W})$ be a strongly continuous group homomorphism which extends to a strongly continuous unitary group on the Hilbert space $\mathcal{H}$, which is l^2_d in this case. Let K be a compact subset of G containing the identity e, and symmetric, $K = K^{-1}$. Clearly $\{ U_k : k \in K \}$ is a simply bounded subset of $\mathcal{L}(\mathcal{W})$ and so, since $\mathcal{W}$ is Fréchet, is equicontinuous. Then for any continuous seminorm p on $\mathcal{W}$ we can find a continuous seminorm q on $\mathcal{W}$, depending on p and K, such that

$$p\left[(U_g - 1)\, x\right] \leq q(x), \qquad g \in K,\ x \in \mathcal{W}.$$

In particular, this means that we can find a positive constant A and a natural number k, depending on p and K, such that

$$p\left[(U_g - 1)\, e_{\mathbf{n}}\right] \leq q(e_{\mathbf{n}}) \leq A\left(|\mathbf{n}| + 1\right)^k, \qquad g \in K,\ \mathbf{n} \in \mathbb{N}^d.$$

Define a function $F : K \to [0, \infty)$, depending on p and K, by setting

$$F(g) = \sum\nolimits_{\mathbf{n}} \frac{p\left[(U_g - 1)\, e_{\mathbf{n}}\right]}{\left(|\mathbf{n}| + 1\right)^{k+2}}, \qquad g \in K.$$

Note that $F(e) = 0$, and

$$0 \leq F(g) \leq \sum\nolimits_{|\mathbf{n}| \leq N} p\left[(U_g - 1)\, e_{\mathbf{n}}\right] + \sum\nolimits_{|\mathbf{n}| > N} A\left(|\mathbf{n}| + 1\right)^{-2}$$

for $g \in K$ and $N \in \mathbb{N}$.

It follows that for any $\epsilon > 0$ we can find a neighbourhood V_ϵ of the group identity e such that

$$g \in V_\epsilon \bigcap K \qquad \text{implies} \qquad F(g) < \epsilon.$$

This shows that F is continuous at e.

We also observe that for all $g \in K$ and all $x \in B_v$,

$$p\left[(U_g - 1)\, x\right] \leq \sum |z_{\mathbf{n}}| v_{\mathbf{n}} p\left[(U_g - 1)\, e_{\mathbf{n}}\right] \leq F(g) \sum v_{\mathbf{n}} \left(|\mathbf{n}| + 1\right)^{k+2}.$$

Choose bounded subsets B, C of $\mathcal{W}$ and $a \in \mathcal{L}^+(\mathcal{W})$. Let v be such that $B \subseteq B_v$. Let w be such that $aB_v \subset B_w$. First we find a continuous seminorm p on $\mathcal{W}$ such that

$$\|x\| + \|ax\| \leq p(x),$$

using the Hilbert space norm. Recall that the left side is a graph norm.

Second, we compute that

$$\begin{aligned}
&\left|\langle y, U_g a U_{g^{-1}} x\rangle - \langle y, ax\rangle\right| \\
&\quad \leq \left|\langle U_{g^{-1}} y, a\left(U_{g^{-1}} - 1\right) x\rangle\right| + \left|\langle\left(U_{g^{-1}} - 1\right) y, ax\rangle\right| \\
&\quad \leq \|y\| \left[\left\|a\left(U_{g^{-1}} - 1\right) x\right\| + \|(U_g - 1)\, ax\|\right] \\
&\quad \leq \sup_C \|y\| \left[p\left((U_{g^{-1}} - 1)x\right) + p((U_g - 1)ax)\right] \\
&\quad \leq \sup_C \|y\| \left\{\left[\sum v_n(|n| + 1)^{k+2}\right] F(g^{-1}) + \left[\sum w_n(|n| + 1)^{k+2}\right] F(g)\right\}
\end{aligned}$$

for all $x \in B$, $y \in C$, and $g \in K$.

It follows from this inequality that we can find a positive constant L, depending on B, C, K and a, such that

$$p_{B,C}(\alpha_g a - a) \leq L\left[F(g) + F(g^{-1})\right], \qquad g \in K.$$

If (g_ι) is a net in K converging to the group identity e, then this last inequality implies that

$$\alpha_{g_\iota} a \to a$$

in $\mathcal{L}^+(\mathcal{W})$.

As we are considering only metrisable groups, it is sufficient to prove that

$$\alpha_{g_m} a \to a$$

in $\mathcal{L}^+(\mathcal{W})$ whenever (g_m) is a sequence in G converging to the identity. But the closure of the set

$$\{g_m : m \in \mathbb{N}\} \bigcup \{g_m^{-1} : m \in \mathbb{N}\}$$

is a symmetric compact subset of G containing the identity. We may substitute this closure for the set K above, and conclude that $\alpha(G)$ is a continuous automorphism group of $\mathcal{L}^+(\mathcal{W})$. ■

Certain automorphisms are of particular interest in physics. The next examples, together with the dynamics, are the principal ones.

6.17 Space Translations We ignore spin and statistics for simplicity. Our wave function space is then $\mathcal{W} = \mathcal{S}\left(\mathbb{R}^{3N}\right)$, and $\mathcal{A} = \mathcal{L}^{+}(\mathcal{W})$.

$\mathbb{R}^3$ acts as a continuous group of isomorphisms of $\mathcal{W}$ through

$$U_a : f \to f_a, \tag{6.35.a}$$

where

$$f_a(x_1, \ldots, x_n) = f(x_1 - a, \ldots, x_n - a), \qquad (a \in \mathbb{R}^3). \tag{6.35.b}$$

These are known as the space translations on $\mathcal{W}$. They are effected by the group

$$U_a = \bigotimes_{j=1}^{N} \exp\left(-ia \cdot p_j\right) \tag{6.35.c}$$

determined by the momentum operators.

It is known from the Weyl relations that $U\left(\mathbb{R}^3\right)$ is continuous on $\mathcal{W}$ and extends to a strongly continuous unitary group on $\mathcal{A}$. It therefore determines a continuous inner automorphism group of the algebra of observables, written $\sigma\left(\mathbb{R}^3\right)$ and also known as the space translations.

There are no space translationally invariant functionals on $\mathcal{A}$.
For as we mentioned above Proposition [6.11], an ergodic state is pure. Exactly as for the time translations, such a state must be formed from an eigenvector of $U\left(\mathbb{R}^3\right)$ in $\mathcal{W}$ — and there are no such functions. Hence there are no ergodic states. Moreover, by Proposition [6.32] below, a general invariant state can always be decomposed into ergodic states, hence the conclusion.

The generalized eigenvectors of $U\left(\mathbb{R}^3\right)$ are the exponentials

$$x \mapsto \exp\left(i\sum_{j=1}^{N} k_j x_j\right), \qquad \left(k_j \in \mathbb{R}^3\right). \tag{6.36}$$

As these distributions are not square integrable, they define generalized states. ∎

6.18 Momentum Translations We continue with the notation of the previous example.

Recall that the Fourier transform may be viewed as a continuous map $\mathcal{F} : \mathcal{W} \to \mathcal{W}$ which extends to a unitary map on $L^2\left(\mathbb{R}^{3N}\right)$. This means that $\mathcal{F}$ determines an implemented automorphism of $\mathcal{A}$,

$$a \to \mathcal{F}\, a \mathcal{F}^{*}. \tag{6.37}$$

Let us apply this automorphism to the space translation group $U(\mathbb{R}^3)$. We shall write

$$V_a = \mathcal{F}\, U_a\, \mathcal{F}^* \tag{6.38.a}$$

for all $a \in \mathbb{R}^3$. It is the fundamental property of $\mathcal{F}$ that

$$V_a = \bigotimes_{j=1}^{N} \exp\left(ia \cdot q_j\right), \tag{6.38.b}$$

where

$$[\mathcal{F}^* V_k f](k_1, \ldots, k_n) = [\mathcal{F}^* f](k_1 - k, \ldots, k_n - k), \qquad (k \in \mathbb{R}^3). \tag{6.38.c}$$

We shall refer to the corresponding unitarily implemented automorphism group $\mu(\mathbb{R}^3)$ on $\mathcal{L}^+(\mathcal{W})$ as the momentum translations.

A functional on $\mathcal{A}$ determined by the $\mathcal{W}$-nuclear operator ρ is invariant under $\mu(\mathbb{R}^3)$ if and only if its transform $\mathcal{F}\,\rho\,\mathcal{F}^*$ is invariant under $\sigma(\mathbb{R}^3)$. Not surprisingly, then, there are no functionals invariant under the momentum translations. ∎

6.19 The Gauge Group We continue with $\mathcal{W}$ as above. Let M_j be the number operator for the j-th coordinate, $1 \leq j \leq 3N$. The group of the torus, T^1, acts on $\mathcal{W}$ through

$$\Gamma_\theta = \bigotimes_{j=1}^{3N} \exp\left(i\theta M_j\right). \tag{6.39}$$

The resulting unitarily implemented automorphism group, $\gamma(T^1)$, is known as the gauge group. The actions of the Γ_θ on $\mathcal{W}$ are known as gauge transformations of the first kind. Every Hermite function determines a pure state which is $\gamma(T^1)$-invariant.
∎

6.20 Dynamical Symmetries If a state T is invariant under an automorphism, it does not follow that its time evolutes T_t are. Group invariance as we have defined it, then, has a static character. We shall say that an automorphism group $\alpha(G)$ is a dynamical symmetry if, whenever a functional T is G-invariant, so are the T_t.

For this to happen, the α_g must commute with the τ_t. In the cases where α is unitarily implemented by, say $V(G)$, all V_g must commute with all U_t. The spectral projections of V, therefore, are functions of the Hamiltonian.

For a general Hamiltonian, none of the three symmetry groups above is a dynamical symmetry. For the free Hamiltonian, the space translations are, and for the harmonic oscillator Hamiltonian, the gauge group is. ∎

6.21 Space Reflections Consider an N particle system in $\mathbb{R}^3$, and let $\mathcal{W}$ include the appropriate spin and statistics. In an obvious notation, consider the operator

$$[\mathcal{R}f] = f(-x_1, s_1; \ldots; -x_N, s_N). \tag{6.40}$$

$\mathcal{R}$ is known as the space reflection operator. Note that the spins are not reversed.

We have remarked before that when spin and statistics are included, the potential function $\mathcal{V}$ must be invariant under $\mathcal{R}$. As usual, we assume that $\mathcal{V}$ does not depend on the spin or velocity.

It follows that for such systems, $\mathcal{R}$ commutes with the Hamiltonian on $\mathcal{W}$. That is, it is a dynamical symmetry. ■

6.6 IMPLEMENTIBILITY

The automorphism groups introduced in the last section were all inner and continuous, and we used the term unitarily implemented to describe this situation. There is another usage for this term, namely if a similar situation occurs in the GNS representation determined by a state.

There is no general necessary and sufficient condition for this to be the case. A sufficient but not necessary condition is that the state in question be invariant under the automorphism (group). When this is so, the left kernel of the state is invariant under the automorphism (group), and this allows the definition of a unitary operator (group) on the quotient space. It is still necessary to examine continuity with respect to the locally convex topologies involved. The next proposition gives the required analysis.

6.22 Proposition Let G be a topological group and $\alpha(G)$ a continuous automorphism group on a unital topological *-algebra, $\mathcal{A}$. Let T be an $\alpha(G)$–invariant state on $\mathcal{A}$, and let $[D, \pi, \Omega]$ be its GNS representation. There exists a strongly continuous unitary representation $U(G)$ of G on D such that

$$U_g D \subset D, \tag{6.41.a}$$

$$U_g \Omega = \Omega, \tag{6.41.b}$$

$$\pi(\alpha_g a) = U_g \pi(a) U_g^* \tag{6.41.c}$$

for all $g \in G$ and all $a \in \mathcal{A}$.

Proof Recall that we write $[a]$ for the image in D of $a \in \mathcal{A}$ under the canonical projection $\mathcal{A} \to \mathcal{A}/L$. By L we mean the closed left ideal in $\mathcal{A}$ containing all elements for which

$$T(a^*a) = 0.$$

The mapping

$$U_g[a] = [\alpha_g a]$$

defines an operator from D into $\mathcal{H}$. Clearly each U_g is isometric. Then L is stable under $\alpha(G)$, from which it follows that D must be as well.

The definition of U guarantees that

$$U_g^{-1} \subset U_g^*,$$

and $g \to U_g$ is a group homomorphism. Then $U(G)$ extends to a unitary representation on $\mathcal{H}$.

The continuity of $\alpha(G)$ ensures that $\langle \xi, U_g\eta \rangle$ is a continuous function on G for all ξ, $\eta \in D$. We can use this to extend U to a strongly continuous unitary group on $\mathcal{H}$. The technique is standard. First consider any vector $\psi \in \mathcal{H}$. Given any $\epsilon > 0$, choose a vector $\xi \in D$ such that

$$\|\psi - \xi\| \leq \epsilon.$$

Hence for any $\eta \in D$,

$$\begin{aligned} |\langle \psi, U_g\eta \rangle - \langle \psi, U_h\eta \rangle| &\leq |\langle \psi - \xi, U_g\eta \rangle| + |\langle \xi, U_g\eta \rangle - \langle \xi, U_h\eta \rangle| + |\langle \psi - \xi, U_h\eta \rangle| \\ &\leq \epsilon\|\eta\| + |\langle \xi, U_g\eta \rangle - \langle \xi, U_h\eta \rangle| + \epsilon\|\eta\|. \end{aligned}$$

The middle term can be made as small as desired as the function in question is continuous on D. Hence $g \to \langle \xi, U_g\eta \rangle$ is continuous for all $\xi \in \mathcal{H}$ and $\eta \in D$.

If we consider this function as a linear functional of η, we may invoke the Riesz–Fréchet theorem to define a vector $\lambda_g \in \mathcal{H}$ depending on g and ξ, such that

$$\langle \xi, U_g\eta \rangle = \langle \lambda_g, \eta \rangle.$$

We can use the same procedure again, and conclude that $g \to \langle \xi, U_g\eta \rangle$ is continuous for all ξ, $\eta \in \mathcal{H}$.

Then for all $\xi \in \mathcal{H}$,

$$\|U_g\xi - U_h\xi\|^2 = \langle \xi, (2 - U_{h^{-1}g} - U_{g^{-1}h})\, \xi \rangle.$$

As $h \to g$ this converges to 0, proving the strong continuity of $U(G)$.

Directly from the definition we see that Ω is invariant, and the covariance equation (6.41.c) holds strongly on D, and we are done. ∎

For normed algebras, the fact that each $\pi(a)$ is bounded allows an extension of the covariance equation from D to $\mathcal{H}$. The above is therefore equivalent to the usual result for C^*-algebras.

We now turn to the question of the existence of invariant states in this general algebraic setting. In order to have a reasonable theory, until further notice we shall assume that the group G is locally compact, separable, and amenable.

Amenability implies the existence of a two sided invariant mean, η, on the space $\mathcal{C}_b(G)$ of bounded and continuous functions from G to $\mathbb{C}$, cf, Greenleaf [1].

In this regard we must mention the following deep result of Johnson [1]. No variant of this for non–normed function spaces over G is known to us.

6.23 Johnson's Theorem A Banach algebra $\mathcal{A}$ is said to be amenable if its first cohomology group $\mathbb{H}^1(\mathcal{A}, X^*)$ vanishes for all Banach $\mathcal{A}$-modules X.

Then G is amenable if and only its group algebra $L^1(G)$ is. ■

We return to the general case. If T is a state and $\alpha(G)$ a continuous automorphism group on $\mathcal{A}$, then

$$F_a(g) = T(\alpha_g a)$$

is evidently continuous for all $a \in \mathcal{A}$.

In the special case where $\mathcal{A}$ is a C^*-algebra, all C^*-homomorphisms are norm decreasing. It follows that

$$|F_a(g)| \leq \|a\|,$$

and so $F \in \mathcal{C}_b(G)$.

Applying an invariant mean, we conclude that

$$\eta(F_a) = \tilde{T}(a)$$

defines an invariant state $\tilde{T}$. This proves the existence of invariance states for C^*-algebras.

For locally convex algebras in general, F_a is continuous but not necessarily bounded. As it is an open question whether or not an invariant mean exists on $\mathcal{C}(G)$, the above method cannot be applied. For such cases, equicontinuity of the automorphism group is sufficient to overcome this difficulty.

After we prove this, we shall consider the question of ergodicity, a topic of particular importance for quantum field theory. The analysis is helped there by the fact that the algebras in question are barreled. For this reason, we shall include some results which require this condition. For an introduction to the theory of equicontinuous groups on locally convex spaces, see Yosida [1].

6.24 Proposition (a) For a barreled topological algebra, every weakly continuous representation is strongly continuous.

(b) For any positive functional T on a barreled *- algebra, the function $a \to T(a^*a)^{1/2}$ is a continuous seminorm, known as a state seminorm. Note that positivity is with respect to the algebraic cone. We assume it to be proper and generating in what follows.

Proof (a) We start from a representation $[D,\ \pi]$ of $\mathcal{A}$ which is weakly continuous, meaning that the function

$$F_{u,v}(a) = \langle u, \pi(a)v\rangle$$

is continuous for each pair of vectors in D.

By the Riesz–Fréchet theorem, since D is dense in $\mathcal{H}$, for any $u \in D$ we observe that the set

$$\{\, a : \|\pi(a)\xi\| \leq 1\,\} = \bigcap\nolimits_{\eta\in D,\, \|\eta\|\leq 1} \{\, a : |\langle \eta, \pi(a)\xi\rangle| \leq 1\,\}\,.$$

As π is weakly continuous, $\{\, a : \|\pi(a)\xi\| \leq 1\,\}$ is closed and absolutely convex. Clearly it is also absorbing, and so is a neighbourhood of 0 in $\mathcal{A}$. This means that we can find a continuous seminorm p_u on $\mathcal{A}$ such that

$$\|\pi(a)u\| \leq p_u(a), \qquad a \in \mathcal{A}.$$

(b) Let T be a continuous positive functional on $\mathcal{A}$. As the product on $\mathcal{A}$ is separately continuous, the GNS representation $[D,\ \pi,\ \Omega]$ is weakly continuous, so strongly continuous by (a). Hence the seminorm

$$T(a^*a)^{1/2} = \|\pi(a)\Omega\|$$

is continuous. ■

Now to the existence theorem.

6.25 Proposition Let $\alpha\,(G)$ be an equicontinuous automorphism group of a locally convex unital *-algebra $\mathcal{A}$. Then the set of invariant states is non empty.

Proof Let T be a continuous positive functional on $\mathcal{A}$, and let us write $T_g = T \circ \alpha_g$. Equicontinuity then implies the existence of a continuous seminorm q such that

$$|T_g(a)| \leq q\,(a)\,, \qquad a \in \mathcal{A},\ g \in G.$$

Since $g \mapsto \alpha_g(a)$ is continuous for any $a \in \mathcal{A}$, the map $g \mapsto T_g(a)$ is continuous. Hence it is an element of $\mathcal{C}_b(G)$. The proof now proceeds as for normed algebras, yielding a G-invariant positive linear functional $\tilde{T}$ on $\mathcal{A}$ such that

$$\left|\tilde{T}(a)\right| \leq K\, q(a)\,, \qquad a \in \mathcal{A},$$

for some constant K. ■

6.7 ERGODICITY

The notion of the state of a system first arose in statistical mechanics. Associated with a state are the phenomena caused by fluctuations. For example, density fluctuations which occur in the liquid–gas transition.

One measure of these fluctuations is the two point correlation function $T_\beta(\rho_x \rho_y)$, where T_β is the state at inverse temperature β, and ρ_x is the density at the point $x \in \mathbb{R}^3$. The basic measure of the collective behaviour of the system is the difference

$$|T_\beta(\rho_x \rho_y) - T_\beta(\rho_x) T_\beta(\rho_y)|.$$

For temperatures above the transition to the gaseous state, this function converges to zero exponentially as $|x - y| \to \infty$. We say that T_β has the cluster property with respect to spatial translations. Similar clustering holds for the n-point correlation functions as well.

Further analysis of such problems led Wiener to conjecture that amongst the set of equilibrium states, the extremals were distinguished by the clustering property. This has been borne out by subsequent work on statistical mechanics, cf, Bratteli and Robinson [1], Dubin [1], Emch [1], Glimm and Jaffe [1], Israel [1], Ruelle [1].

For normed algebra models of statistical mechanics, a more or less satisfactory theory of this connection is known. For unbounded operator algebras, the situation is less good. In this section we shall indicate what can be done in a fairly general setting. This material is rather technical, and we omit most of the proofs. These can all be found in Alcantara-Bode [1] and, in abbreviated form, in Alcantara-Bode and Dubin [1]. Note that Proposition (6.32) was used previously.

Let us introduce the following convention. All algebras $\mathcal{A}$ in this section shall be unital topological *-algebras with a proper positive algebraic cone. We shall assume given a continuous symmetry group of automorphisms $\alpha(G)$ which preserves positivity.

We also assume that if T is a state, then the Hilbert space closure $\mathcal{H}$ of the GNS domain D is separable. This is so if the topology of $\mathcal{A}$ is separable, eg, if it is second countable. Not all of these conditions are necessary for the results below, but they hold in all cases of physical interest.

6.26 Proposition Let T be a G-invariant state on $\mathcal{A}$. Consider the following conditions

(i) T is G-ergodic.

(ii) Let $\mathcal{B}_T$ be the family of operators

$$\mathcal{B}_T = \pi(\mathcal{A}) \bigcup U(G)\,|_D,$$

acting on the domain D. Then $(\mathcal{B}_T, D)'_w = \mathbb{C}$.

(iii) The range of P, the orthogonal projection onto the set of $U(G)$-invariant vectors in $\mathcal{H}$, is one dimensional and spanned by the GNS cyclic vector $[\mathbf{1}]$.

Then the following implications hold:

$$(i) \iff (ii) \implies (iii).$$

Proof This proposition may be considered an extension of [**3.33**], and the reader is reminded of the reference Powers [1].

$(i) \implies (ii)$. Assume $(\mathcal{B}_T, D)'_w \neq \mathbb{C}$. Then as in Powers [1], we can show that there exists an element $L \in (\mathcal{B}_T, D)'_w$ such that L is not scalar, $0 \leq L \leq \mathbf{1}$ and

$$\langle [\mathbf{1}], L[\mathbf{1}] \rangle \neq 0.$$

Now

$$T_1(a) = \langle [\mathbf{1}], \pi(a) L[\mathbf{1}] \rangle / \langle [\mathbf{1}], L[\mathbf{1}] \rangle$$

and

$$T_2(a) = \langle [\mathbf{1}], \pi(a)(1 - L)[\mathbf{1}] \rangle / \langle [\mathbf{1}], (1 - L)[\mathbf{1}] \rangle$$

are G-invariant states such that $T_1 \neq T_2$.

With $\lambda = \langle [\mathbf{1}], L[\mathbf{1}] \rangle$, moreover,

$$T = \lambda T_1 + (1 - \lambda) T_2.$$

$(ii) \implies (i)$. Suppose there exist G-invariant states T_1 and T_2 and a number $0 < \lambda < 1$ such that

$$T = \lambda T_1 + (1 - \lambda) T_2.$$

Then, Powers [1], there exists an $L \in (\mathcal{B}_T, D)'_w$ which is not scalar, bounded by $0 < L < \lambda \mathbf{1}$, and

$$\lambda T_1(a^* b) = \langle [a], L[b] \rangle.$$

We omit the proof of the last implication, which can be found in the thesis of Alcantara-Bode [1]. ∎

There does not seem to be a reasonable condition known which will assure that the reverse implication $(ii) \Longleftarrow (iii)$ holds in general. The link between clustering and extremal states is the notion of asymptotic abelianness. The natural form this takes in the general case seems to be in the weak sense. To save writing we shall abbreviate the term "weakly asymptotically abelian" to waa.

6.27 Definition A state T on $\mathcal{A}$ is said to be weakly asymptotically abelian with respect to $\alpha(G)$ if for every pair of vectors $u, v \in D$, every pair $a, b \in \mathcal{A}$, and every $\varepsilon > 0$, there exists a compact subset Δ of G such that for all $g \in G \backslash \Delta$,

$$\left|\langle v, [\pi(\alpha_g a), \pi(b)]_- u\rangle\right| < \varepsilon. \tag{6.42.a}$$

■

Note that a waa state need not be G-invariant. We can rewrite equation (6.42.a) directly in terms of the state:

$$\left|T\left(c^*[\alpha_g a, b]_- d\right)\right| < \varepsilon, \tag{6.42.b}$$

for all a,b,c,$d \in \mathcal{A}$, and $g \in G/\Delta$. Note the general commutator notation

$$[x, y]_- = xy - yx.$$

6.28 Lemma For a G-invariant waa state T on a locally convex algebra $\mathcal{A}$, the function

$$F(g) = \|\pi(a)U_g[b]\| \tag{6.43.a}$$

is an element of $\mathcal{C}_b(G)$ for all a and $b \in \mathcal{A}$.

Proof F is written in our standard GNS notation. In terms of T itself,

$$F(g) = T\left(b^*\alpha_{g^{-1}}(a^*a)b\right)^{1/2}. \tag{6.43.b}$$

We know that F is continuous, just as in Proposition [6.25].

Consider the estimate

$$F(g)^2 \le \left|T\left(b^*[\alpha_g(a^*a), b]_-\right)\right| + |T(b^*b\alpha_g(a^*a))|.$$

Given $\epsilon > 0$, we can find a compact set $\Delta \subset G$ such that for g in the complement of Δ, the first term is less than ϵ. Hence the first term is bounded on G.

The second term is bounded by

$$|T(b^*b\alpha_g(a^*a))| \le T(a^*a\,a^*a)^{1/2}\; T(b^*b\,b^*b)^{1/2},$$

by using the Cauchy–Schwarz inequality and G-invariance. ■

As the operators $\pi(a)$ are unbounded in general, certain domain questions arise. In particular, it is important to know the action of the projection operator P on D.

The reader will recall the definitions of the adjoint representations (π^*, D^*) and (π^{**}, D^{**}) in Definition (3.32).

The next results are due to Alcantara-Bode, and the reader is referred for a proof to the references above.

6.29 Proposition Let T be a G-invariant waa state on a barreled algebra $\mathcal{A}$.

(a) Then

$$P\,D \subset D^{**}.$$

(b) If T is G-invariant but not necessarily waa, the domains D^* and D^{**} are invariant under $U\,(G)$. In addition, $U\,(G)$ acts covariantly on the representation,

$$U_g \pi^{\diamondsuit}(a) U_g^* v = \pi^{\diamondsuit}(\alpha_g a) v$$

for all g, a, and all $v \in D^{\diamondsuit}$. Here $\diamondsuit$ stands for $*$ or $**$.

(c) If T is G-invariant and waa, then for every a, $b \in \mathcal{A}$, every v, $w \in D^{**}$ and $\epsilon > 0$, there exists a compact subset Δ of G such that for all $g \in G \backslash \Delta$,

$$\left| \langle [\pi^{**}(\alpha_g a), \pi^{**}(b)]_- \, u, v \rangle \right| < \epsilon.$$

(d) The reduced family $\{\, P\pi^{**}(a)P : a \in \mathcal{A} \,\}$ is a strongly abelian op* – algebra on D^{**}. By strongly abelian we mean

$$[P\pi^{**}(\alpha_g a)P, P\pi^{**}(b)P]_- \, u = 0$$

on D^{**}. ■

We have shown that every state may be decomposed into pure states. We have mentioned that every invariant state may be decomposed into ergodic states. A proof of this is our next topic. Note that by taking the group to be $\{\, e \,\}$, the original decomposition into pure states results.

For a C^*-algebra one is in the happy position that the set of states is compact in the $\sigma\,(\mathcal{A}', \mathcal{A})$ topology. This enables one to apply the Choquet theory of simplicial decomposition, cf, Choquet [1], Sakai [1]. For locally convex algebras this is not generally possible.

Borchers and Yngvason [1,2] have developed a decomposition theory for op* – algebra, based on a transfinite construction of positivity preserving extensions. Mathot

[1] has developed a method which applies to barreled algebras with a certain countability property.

The result we shall give is due to Hegerfeldt [1], who made the ingenious observation that by considering a countable dense subalgebra, standard simplex theory applies to its algebraic dual. The resulting decomposition is then shown to restrict to the dual of the original algebra. We change our convention in that the algebra $\mathcal{A}$ will have only the properties indicated in the theorems.

6.30 Lemma Let $\mathcal{A}$ be a unital *-algebra which is the finite linear span of a countable subset

$$\mathcal{B} = \{ b_1, \dots, b_n, \dots \}$$

of $\mathcal{A}$. Let $\mathcal{A}^*[\sigma^*]$ be the algebraic dual of $\mathcal{A}$, equipped with the weak topology

$$\sigma^* = \sigma(\mathcal{A}^*, \mathcal{A}) .$$

Then, if we define positivity on $\mathcal{A}$ through the algebraic cone, assumed proper, the positive cone $\mathcal{A}^*_+$ is proper, metrizable and complete.

Proof For each $b \in \mathcal{B}$, let p_b be the seminorm in $\mathcal{A}^*$ whose closed unit semiball is

$$\{ T \in \mathcal{A}^* : |T(b)| \leq 1 \} .$$

As $\mathcal{B}$ is linearly generating, the countable family $\{ p_b : b \in \mathcal{B} \}$ generates σ^*. Hence σ^* is metrizable. As $\mathcal{A}^*$ contains all linear functionals on $\mathcal{A}$, continuous or not, $\mathcal{A}^*$ and $\mathcal{A}^*_+$ are σ^* complete. Finally, $\mathcal{A}^*_+$ is proper because $\mathcal{A}$ is unital. ∎

Now we prove the decomposition theorem into ergodic states. This was referred to in earlier work.

6.31 Proposition Let T be a state on a unital nuclear *–algebra $\mathcal{A}[t]$ with proper algebraic positive cone $\mathcal{P}(\mathcal{A})$. Suppose the topology is such that the state seminorm

$$p_T(a) = T(a^* a)^{1/2}$$

is continuous. This is the case, for example, if it is barreled. There exists a standard measure space Z, a weakly measurable map $z \to T_z$ from Z to the extremal states on $\mathcal{A}$, and a probability measure μ on Z such that

(i) $$T = \int_Z^{\oplus} T_z \, d\mu(z);$$

(ii)
$$[a] = \int_Z^{\oplus} [a]_z \, d\mu(z);$$

(iii) the left kernels satisfy $L(T) \subset L(T_z)$ for μ-almost all z. (iv) Let G be a topological group containing a dense countable subgroup, and acting on the algebra through a continuous group of automorphisms. If T is G-invariant, the $\{T_z\}$ can be taken to be ergodic for μ-almost all z; and the unitary groups decompose in accordance with

$$U(g) = \int_Z^{\oplus} U_z(g) \, d\mu(z).$$

Proof (1) We break the proof into a number of steps. For any continuous seminorm p we write $\mathcal{A}_p$ for the norm completion of $\mathcal{A}/\mathrm{Ker}(p)$. There is no loss of generality in taking p to be Hilbertian, as $\mathcal{A}$ is nuclear. Then $\mathcal{A}_p$ is a Hilbert space. By $\mathcal{A}[p]$ we mean the algebra $\mathcal{A}$ equipped with the psuedometric topology obtained from p. As $\mathcal{A}$ is barreled, a state T determines a continuous seminorm

$$p_T(a) = T(a^* a)^{1/2}.$$

Nuclearity implies that given p, there exists a continuous seminorm $q \geq p$ such that the canonical map $\mathcal{A}_q \to \mathcal{A}_p$ is surjective and nuclear; and that $\mathcal{A}[q]$ is separable.

(2) As $\mathcal{A}[q]$ is separable, choose a q-dense countable subset $\mathcal{B}_1 \subset \mathcal{A}$ containing the identity and such that $\mathcal{B}_1 \bigcap \mathcal{P}(\mathcal{A})$ is dense in $\mathcal{P}(\mathcal{A})$. Let G_0 be a dense countable subgroup of G, and let $\mathcal{B}$ be the *–algebra generated by $\alpha(G_0)\mathcal{B}_1$. It is spanned by a countable set, contains the identity, and $\mathcal{B} \bigcap \mathcal{P}(\mathcal{A})$ is q-dense in $\mathcal{P}(\mathcal{A})$.

Let T' be the state T restricted to $\mathcal{B}$, and (π', D', Ω') the GNS representation obtained from it. As T' is $\alpha(G_0)$-invariant, $\alpha(G_0)$ is unitarily implemented by a strongly continuous group $U'(G_0)$ in the representation. Note that for all $g \in G_0$,

$$U'(g)\Omega' = \Omega'.$$

(3) Consider the *-algebra $\mathcal{C}$ generated by the union $\pi'(\mathcal{B}) \bigcup U'(G_0)$. By construction, $\mathcal{C}$ is spanned by a countable set and contains the identity. It is a *-subalgebra of $\mathcal{L}^+(D')$, and so its algebraic cone is proper.

The previous lemma applies to $\mathcal{C}$: $\mathcal{C}^*_+[\sigma(\mathcal{C}^*, \mathcal{C})]$ is proper, metrisable and complete.

(4) We now define a state T'' on $\mathcal{C}$ by setting

$$T''(c) = \langle \Omega', c\,\Omega' \rangle, \qquad c \in \mathcal{C}.$$

Note that T'' restricted to $\mathcal{B}$ is just T'.

The properties of $\mathcal{C}^*$ just noted imply that there is a cap K containing T'' and a maximal Radon measure $m \in \mathcal{M}^1(K)$ for which T'' is the resultant. The measure m is supported by the extreme rays of $\mathcal{B}^*_+$. Note that the extreme states constitute a G_δ-set. Thus

$$T'' = \int_{Z'}^{\oplus} T''_z \, d\mu'(z)$$

for some standard measure space Z' and probability measure μ'. In this decomposition we have normalized the T''_z, and in compensation scaled m to μ'.

The quantities comprising the GNS representation for T'' also decompose. Noting that if $c = \pi'(b)$, then $\pi''(c) = \pi'(b)$; and if $c = U'(g)$, then $\pi''(c) = U'(g)$. Note that $D'' = D'$ and $\Omega'' = \Omega'$. Thus we arrive at the integral decompositions

$$D' = \int_{Z'}^{\oplus} D'_z \, d\mu'(z),$$

$$\pi' = \int_{Z'}^{\oplus} \pi'_z \, d\mu'(z),$$

$$\Omega' = \int_{Z'}^{\oplus} \Omega'_z \, d\mu'(z),$$

and

$$U'(g) = \int_{Z'}^{\oplus} U'_z(g) \, d\mu'(z).$$

As Ω' is G_0-invariant, it follows easily that almost all Ω'_z are. Hence almost all T''_z are irreducible and $\alpha(G_0)$-invariant.

The algebra $\mathcal{C}$ has been used only in order to obtain these decompositions. It will play no role hereafter. We need only consider the primed quantities and extend them from G_0 to G and $\mathcal{B}$ to $\mathcal{A}$.

(5) Now we start the extension process. The first extension is painless. If $b \in \mathcal{B}$, then $[b] = [b]'$, so the D' decomposition holds for those vectors in $\mathcal{H}$ of this form.

For an arbitrary $a \in \mathcal{A}$, let (b_n) be an $\mathcal{B}$-sequence converging to a in the q topology. Then

$$\|[a] - [b_n]'\| = p(a - b_n) \leq q(a - b_n).$$

It follows that we may complete the D' decomposition in the Hilbert topology. Then

$$\mathcal{H} = \int_{Z'}^{\oplus} \mathcal{H}'_z \, d\mu'(z).$$

Then for all $a \in \mathcal{A}$ we can write

$$[a] = \int_{Z'}^{\oplus} F(a, z)\, d\mu'(z).$$

Now $a \to [a]$ is strongly continuous $\mathcal{A}[q] \to \mathcal{H}$. By the nuclear spectral theorem, the same holds for the function $a \to F(a, z)$ for all $z \in Z'$.

For each $b \in \mathcal{B}$,

$$F(b, z) = \pi'_z(b)[\mathbf{1}]'_z = [b]'_z$$

for all z save in a b-dependent μ'-null set. Write N for the union over all $b \in \mathcal{B}$ of these sets; then N is a μ'-null set. Morover, this last equation is then true for all $b \in \mathcal{B}$, all $z \in Z' \backslash N$.

Define

$$T_z(a) = \langle F(a, z), [\mathbf{1}]'_z \rangle$$

for all $a \in \mathcal{A}$ and all $z \in Z'$. For $b \in \mathcal{B}$ and $z \in Z' \backslash N$, the identity

$$T_z(b) = T'_z(b)$$

holds. That is, T'_z is the restriction of the q- continuous functional T_z on $\mathcal{A}$ to $\mathcal{B}$. As $\mathcal{B}_+$ is dense in $\mathcal{P}(\mathcal{A})$, it follows that T_z is positive.

As T'_z is extreme in the state space for $\mathcal{B}$, the weak commutant

$$[\pi'_z(\mathcal{A}), D'_z]'_w = \mathbb{C}.$$

Because π_z extends π'_z, its weak commutant is also scalar. It follows that the T_z are extreme in the state space for $\mathcal{A}[t]$. This argument has enabled us to pass from an extremal decomposition in $\mathcal{B}^*_+[q]$ to one in $\mathcal{A}'_+[t'_b]$. Note that the argument is valid because the state seminorm p_T is continuous.

(6) Consider the extension from G_0 to G. This entails another completion, leading to the decomposition

$$[\alpha_g a] = \int_{Z'}^{\oplus} f(a, g, z)\, d\mu'(z)$$

for all $a \in \mathcal{A}$, $g \in G$.

Restricting to $\mathcal{B}$ and G_0, we identify

$$\langle f(a, g, z), [b]_z \rangle = \langle U'_z(g)[c]_z, [b]_z \rangle$$

outside a μ'-null set. As before, we can construct a single null set N' so that the above equation is true for all pairs a, $b \in \mathcal{B}$ and $g \in G_0$.

Write N'' for the union of N and N'. Then $U'_z(G_0)$ is the restriction of a unitary group $U_z(G)$ for all $z \in Z' \backslash N''$. With the definitions

$$Z = Z' \backslash N'',$$

and

$$\mu = \mu' | Z,$$

we have now constructed the required decomposition.

Now we must show that the inclusion of the symmetry preserves ergodicity. We note that the weak commutants

$$\left[\pi'_z(A) \bigcup U'_z(G_0), D'_z\right]'_w = \mathbb{C}$$

are scalar. By the same argument as above, it follows that

$$\left[\pi_z(A) \bigcup U_z(G), D_z\right]'_w = \mathbb{C}.$$

By the ergodic theorem [6.26], the T_z must be ergodic.

Finally, if $a \in L(T)$,

$$0 = \int_Z T_z(a^* a)\, d\mu(z),$$

implying that $a \in L(T_z)$ for μ-almost all z. ■

Now we are able to complete the proof of the ergodic theorems we have presented for $\mathcal{L}^+(\mathcal{W})$.

6.32 Proposition The decomposition of the previous proposition holds for states on the algebra of observables $\mathcal{L}^+(\mathcal{W})[\mu]$.

Proof Let us write $\mathcal{A}$ for $\mathcal{L}^+(\mathcal{W})$. Then if $T \in \mathcal{A}[\mu]'$ is $\mathcal{K}$–positive, it is certainly $\mathcal{P}(\mathcal{A})$–positive, and $\mathcal{P}(\mathcal{A})$ is known to be proper.

It will prove convenient to equip $\mathcal{A}$ with the quasi–uniform topology τ^* introduced by Lassner [4]. This is the topology of uniform convergence on bounded subsets it inherits from $\mathcal{L}(\mathcal{W})$ rather than $\mathcal{L}(W, W')$. It is determined by the seminorms

$$Q_{p,B}(a) = \max\left[\sup_{x \in B} p(ax), \sup_{x \in B} p(a^+ x)\right],$$

as B runs through the bounded subsets of W and p through the continuous seminorms on W.

Using the symmetry under the adjoint, it is elementary to show that

$$\mathcal{A}[\tau^*] \subset \mathcal{L}(\mathcal{W})_b \bigoplus \mathcal{L}(\mathcal{W})_b .$$

It follows that $\mathcal{A}[\tau^*]$ is nuclear.

The proof that $\mathcal{A}[\mu]$ is separable depended on the existence of the Hermite Schauder basis for W, and can be taken over for this case. That is, $\mathcal{A}[\tau^*]$ is separable.

Now let T be a state on $\mathcal{A}[\mu]$. Using the seminorms of equation (4.11), there exists a positive constant C and a $\mathbf{v} \in \Gamma$, depending on T, such that

$$|T(b)| \leq C\, p_{\mathbf{v}}(b), \qquad b \in \mathcal{A}.$$

Substituting $a^+ a$ for b leads to

$$p_T(a) \leq \max\left[\sup_{x\in B_v} \|ax\|, \sup_{x\in B_v} \left\|a^+ x\right\|\right].$$

Hence p_T is a continuous seminorm on $\mathcal{A}[\tau^*]$.

All the conditions for the previous proposition have been shown to hold for $\mathcal{A}[\tau^*]$. This leads to a decomposition into G–ergodic pure states on $\mathcal{A}[\tau^*]$. Being pure, they are $\mathcal{K}$–positive linear functionals on $\mathcal{A}$, hence continuous on $\mathcal{A}[\mu]$. ■

As the Hilbert space of the system is separable, a self adjoint operator has at most a countable number of orthonormal eigenvectors. For the inner automorphisms of $\mathcal{L}^+(\mathcal{W})$ discussed previously, the ergodic components of an invariant state must be eigenstates. Hence the integral decomposition above must reduce to a sum: the measure must be discrete. Our previous assertions have now been shown. But note that this proposition is not confined to inner automorphism groups.

We have not stated that the measure μ is unique; in general it is not. Klauder (unpublished) has even constructed a state for the canonical commutation relations in quantum field theory which has two extremal decompositions of mutually disjoint support. In view of the physical interpretation of extreme states as pure phases in statistical mechanics, this is a phenomenon worth further analysis.

Thomas [2] has a different approach to decomposition theory. An important result of his concerns the uniquness of the measure.

6.33 Proposition A necessary and sufficient condition for the representing measure to be unique is for the space $\mathcal{A}'_h$ of hermitian functionals to be a lattice in the $\mathcal{A}'_+$-order. ■

7. QUANTUM THEORY OF MEASUREMENTS

7.1 ORIENTATION

The origin of quantum measurement theory was the realization that such a theory was needed at all. That this was so was first of all clear from experiments in which light behaved like particles : the photons of the photoelectric effect (Einstein [1-2]); and experiments in which particles behaved like waves : the diffraction patterns of electrons refracted by metals (Davisson and Germer [1]). Not only do macroscopic concepts like wave–like and particle–like lose their absolute significance, but a deeper truth is exposed. This was emphasized by Bohr [2-3] under the name complementarity. His point was that such qualities were a result of the particular nature of the observation. Nothing could be known without observation, and observation required a non–negligible interaction between observer and observed.

There is an evident division between the formalism of the theory and its interpretation. In the axioms of von Neumann, the formalism is represented by axioms 1, 2 and 5; and the interpretation by 3 and 4. The interpretive axioms have a discontinuous aspect to them, based on a change of state accompanying a measurement. There is also the nonclassical probability aspect, due to Born [2]. Not only does the state change discontinuously, depending on the measured value; but the values allowed are predictible only in a statistical sense.

In this chapter we shall examine the modifications in this usual theory of quantum measurements necessitated by adopting the mathematical scheme described in the previous chapters. In order to delineate what we shall, and shall not, be discussing, we recall here the the physical interpretation of quantum theory alluded to above.

To simplify the discussion we start by considering only self adjoint operators whose essential spectrum is empty, and whose eigenvalues all have unit multiplicity. Let us further assume that the operators in question possess an orthonormal basis of eigenfunctions. We shall refer to such operators as complete simple observables.

Our first caveat, and one we shall continually elaborate, is this. Such an operator is meant to contain all the information about a physical property that quantum mechanics is able to assert. This perfect univocal correspondence cannot seriously be maintained. Between the operators of quantum theory and physical reality lies a set of assumptions, and is in large measure an open question. The most obvious problem here is the definition of reality, and its connection with states of consciousness.

Our algebraic model sheds no light on these problems of reality and consciousness, and so aside from occasional remarks, we shall not discuss them. In spite of the inherent difficulties,then,

we make a terminological commitment by identifying quantum operators with the physical phenomena they represent.

In our terminology, an individual measurement consists of examining an incoming state for the quantal properties represented by the operator, registering the result, and then emitting an outgoing state. If we demand, as we have, that probability be conserved, we preclude consideration of destructive measurements.

An ensemble of individual measurements constitutes a statistical measurement. A statistical measurement is equivalent to a quantum distribution law for the observable in the state. It is the individual measurement which has the physical immediacy, modulo the above caveat. But the implications of an individual measurement require it to stand as a component of a statistical measurement. Classical mechanics does not seem to require such a setting: a measurement of the momentum of a particle is just that, and stands on its own.

It might be prudent to note that we have in mind the measurement of properties which might be termed *variable*, such as position, momentum, or energy. We assume that certain parameters of the system are fixed *a priori*, such as mass and charge. This is no profound restriction, though. Were a modification of the theory to supply a mass or charge operator, their measurements would then be included in the formalism.

Measurements are accomplished by means of instruments. An instrument registers eigenvalues and emits outgoing states accordingly. It results in the registration of a particular eigenvalue. The corresponding outgoing state is an eigenstate for that eigenvalue, independent of the incoming state.

The instrument itself must satisfy certain requirements in order that the process just described accords with our primitive notion of a measurement. First of all it must be capable of a permanent registration of the result. A developed photograph of a particle track is a model process.

Secondly, it must be of macroscopic size. If two particles collide, that is an event, but not a measurement. If a photograph of the event is taken, that is a measurement. If the information obtained refers to only one of the particles, the device consists of the recording apparatus and the other particle as well. If the property being measured refers to both particles, it is the recording apparatus alone that is the instrument.

Our second caveat is now required. It is an open question as to whether or not a consciousness is a necessary part of an instrument. In spite of the fact that we can imagine, say, a camera operating automatically, there are subtle arguments to the effect that a quantum measuring event is not over until it is registered in someone's mind. Fortunately, this problem does not seem to be affected by the choice of algebra, so we refer to the literature. Jammer [2] is a good place to start.

Von Neumann [2] has developed a model of an ideal instrument which can be described in quantum mechanical terms by an operator on the instrument Hilbert space. The macroscopic size of the instrument is taken to mean that the spectrum of the instrument operator has states which behave like a classical pointer. Another sort of model would be for the instrument to be analogous to a reservoir in statistical mechanics. In this case, it is the infinite number of degrees of freedom of the instrument which gives the classical behaviour. An example along these lines has been given by Hepp [1].

Hepp's work is quite important, since he was able to demonstrate that the classical behaviour of the measuring device can be described completely in quantum mechanical terms. This avoids the vaguely regressive aspect in Bohr's description of the measurement process. We note that Hepp's analysis relies on the existence of disjoint representations of operator algebras and of a suitable family of observables, the algebra of observables at infinity.

Let the system under observation and the instrument combined be called the universe. This is only sensible if we can isolate them from everything else. Now the system and instrument are taken to be in interaction for a certain period of time. During this period, the universe evolves according to a unitary group determined by a universe Hamiltonian. Note that pure states of the universe will evolve into pure states.

As when we first discussed states in Chapter 5, it is the projection onto the two subsystems which is of interest. One of the most controversial points in quantum theory concerns precisely this projection.

The canonical view is that the record of the event requires an end to the unitary evolution. The instrument ends up in a classical–like state, perhaps metastable. The system ends up in an eigenstate of the operator being measured. The interaction between the system and instrument provides the correlation between their respective states, which enables us to say, eg : when the pointer is here, the system has such and such an energy.

The controversy concerns the mechanism for the sudden, irreversible, and uncontrollable change from the unitary evolution to these final states. Our model will have something to say about the class of final states available in this process, but not about its cause. For that we must once again refer to the literature, eg, Jammer [2], Von Neumann [2].

In Hepp's work (ibid), the reduction from the quantum to the classical probability law does not require any external cause, such as consciousness. Our inclination is to consider Hepp's work as the correct description of the Cøpenhagen interpretation. It is an open problem to extend his work to our model, and there does not seem to be any particular obstruction to doing so.

In the process described, an individual measurement is seen to be a filter for the eigenprojections of the observable. In a standard terminology, the sudden change from an arbitrary incoming state to an eigenstate will be referred to as the *collapse of the state.* In what follows, we shall be interested only in the behaviour of the state of the system. That an individual measurement results in a collapse of this state will be assumed as an axiom, and left at that. The instruments will be treated as a "black box" with certain modest mathematical properties.

The reader will recall that the only possible instrument readings are the eigenvalues of the observable. If a given eigenvalue is recorded, then the collapsed state is the corresponding eigenstate. It is not generally possible to know in advance which eigenvalue will result from an individual measurement. This predictive uncertainty is another source of misgivings to many people. Einstein was particularly dubious about this, feeling that it indicated an incompleteness of the theory.

Note the assumption that there exist ideal instruments, in principle at least. These instruments give exact eigenvalue readings, and emit undistorted eigenfunctions. Hence if an individual measurement is repeated immediately, the same eigenvalue surely occurs, and the same eigenstate is emitted. This is known as strict repeatability.

An interesting consequence of strict repeatabilitiy is known as state preparation. To create a given pure state, construct an instrument of which the state is an eigenstate. Perform individual measurements on the instrument until the relevant eigenvalue appears. The emitted state is then the one desired.

Suppose an ensemble of individual measurements is made. The resulting statistical measurement consists in the pairing of a particular eigenvalue with a probability of transition from the incoming state to the outcome eigenstate. This is the only place where the incoming state appears.

In our algebraic model, these conclusions will be modified. It will be seen that for most observables, ideal instruments do not exist. This means that strict repeatability is not usually possible. Even more, only partial spectral information can be obtained from a statistical measurement.

For further reading on the quantum theory of measurements, in addition to the works already cited, we recommend Bohm [1], Gillespie [1], Jauch [1], Kemble [1] and Ludwig [1].

In 1970, Davies and Lewis published an important paper examining the measurement process for bounded operators with continuous spectra. As their work serves as a model for ours, it is worth outlining the essence of their idea (Davies and Lewis [1], Davies [1,2]).

Choose $\mathcal{A} = \mathcal{L}(\mathcal{H})$ as the algebra of observables. An instrument is taken to be a black box which accepts incoming states, reads spectral values, and emits a collapsed state. Which state is emitted is contingent upon the spectral value recorded.

Rather than reading eigenvalues only, instruments read spectral intervals, or more generally, Borel subsets of the spectrum. For mathematical convenience, we shall allow our instruments to accept positive linear functionals which are not necessarily normalized. As the positive cone $\mathcal{K}'$ of $\mathcal{A}'$ is generating, linearity suggests that we extend this so that arbitrary elements of $\mathcal{A}'$ are accepted.

Our primitive instrument, then, is a family of linear maps from $\mathcal{A}'$ (incoming) to $\mathcal{A}'$ (outgoing), labelled by the Borel subsets of the observable to be measured, and preserving positivity and normalization. This last requirement implies that states map to states. As a first refinement, a certain σ-additivity over the Borel subsets is required, so as to be compatible with the spectral theorem.

Davies and Lewis find it convenient to take the spectral families obtained from the operators as their notion of observable. This is similar to the point of view adopted by some other writers, notably Ludwig [1]. In view of the Naimark spectral theorem for symmetric operators, they admit as observables positive operator valued measures. An observable representated by a self adjoint operators is then distinguished by a unique spectral decomposition in terms of a projection valued measure (PVM).

Their results are rather interesting. When applied to complete simple observables, the usual results are obtained. This is intuitively clear, as isolated eigenvalues are discernible in the intervals surrounding them. Their eigenprojections are also distinguished by a discontinuity in the spectral measure.

For general observables, things are different. One records spectral intervals, not only points. Away from eigenvalues, the output state is not strictly repeatable, although definite.

In a subsequent paper, Davies [1] considered the measurement of an observable by an instrument correlated to a second observable. The second observable is constructed in a certain way out of part of the spectral measure of the first, and is said to have less information than the first. A measurement with such an instrument gives incomplete information about the observable being measured.

The point of this is that it may not be possible to measure an observable perfectly, but it may be possible to measure it imperfectly in the above sense. Putting together all these imperfect measurements then gives the maximum information possible about the observable. This proves to be the typical situation for unbounded operators, and so this idea, adapted to our model, is of importance in what follows.

It is worth noting that Srinivas [1] has investigated a weakening of the definition of an instrument in the bounded case, so as to retain strict repeatability. He found that this required replacing σ-additivity by finite additivity. Finite additivity is a very limiting axiom for measure theory. In addition, as it does not seem empirically justified, we shall retain the countable additivity in what follows.

7.2 OPERATIONS AND INSTRUMENTS

We now present an adaptation of the Davies and Lewis theory to the choice of $\mathcal{L}^+(W)$ as algebra of observables. This choice incurs essential technical complications not present for $\mathcal{L}(\mathcal{H})$. The material in this chapter is a refinement and extension of the work of Dubin and Sotelo [1] and Sotelo [1].

The natural definition of an instrument would seem to be as a map from the Borel sets of the spectrum into the positive linear maps on $\mathcal{A}'$, with values for different Borel sets fitting together as a measure. Now an instrument is a device to measure a quantum property, as represented by an observable. If this physical interpretation is to be possible, the pre–transpose of an instrument must be a family of linear maps taking observables to observables. Because $\mathcal{A}$ is incomplete, this is not a general property of pre–transposes of elements of $\mathcal{L}\left(\mathcal{A}'\right)$. What we must do is to allow as instruments only those elements of $\mathcal{L}\left(\mathcal{A}'\right)$ whose pre–transposes are elements of $\mathcal{L}(\mathcal{A})$. This makes the definition we adopt a little awkward, but no natural alternative is known to us.

Granting this, we start from the pre-transpose of an instrument, which we call an operation. An instrument, then, will be the transpose of an operation. It is possible to define an operation in such a way that an instrument has just the properties wanted.

We note that in the paper of Dubin and Sotelo [1], this was called an expectation. The terminology now employed is consistent with the work of Davies and Lewis [1], and of Haag and Kastler [1] who first introduced the term.

A second difficulty is associated with the spectral decomposition of elements of $\mathcal{A}_h$. Unless $b \in \mathcal{A}_h$ is essentially self adjoint, it has many different spectral representations by positive operator valued measures (POVM). This is part of the spectral theorem of Naimark discussed previously.

In the other direction, we consider all the POVM which integrate to an element of $\mathcal{A}_h$ in a certain topology. We call these $\mathcal{A}$-measures, and write $\mathcal{M}_+(\mathcal{A})$ for the set of them.

Consider the essentially self adjoint position operator q on $\mathcal{S}(\mathbb{R})$. The spectral decomposition of its closure is unique and well known to be given by

$$\mathcal{E}_q(\Delta) = \kappa_\Delta,$$

the characteristic function of the real Borel set Δ. The family $\{\Delta \to \kappa_\Delta\}$ is thus the unique $\mathcal{A}$-measure associated with q.

It is easy enough to see that there are functions $u \in \mathcal{S}(\mathbb{R})$ such that

$$x \to \kappa_\Delta(x)u(x)$$

is not in $\mathcal{S}(\mathbb{R})$. This example shows that there are $\mathcal{A}$-measures which do not leave the domain $\mathcal{W}$ invariant. For this reason we must consider the subset of $\mathcal{A}$- measures under which $\mathcal{W}$ is stable. We call these $(\mathcal{A},\mathcal{W})$-measures, and write $\mathcal{M}_+(\mathcal{A},\mathcal{W})$ for the set of them. Then

$$\mathcal{M}_+(\mathcal{A},\mathcal{W}) = \mathcal{M}_+(\mathcal{A}) \bigcap \mathcal{A}. \qquad (7.1).$$

It is out of $(\mathcal{A},\mathcal{W})$-measures that we construct our instruments. In this sense, $\mathcal{M}_+(\mathcal{A},\mathcal{W})$ contains all the answerable quantum mechanical questions. We propose, therefore, to call the $(\mathcal{A},\mathcal{W})$-measures *questions*.

Given a single bounded operator, it defines an abelian W^*–algebra in a natural way. This is the algebra of all L^∞ functions on its spectrum. Conversely, every abelian W^*–algebra is equivalent to such a function space.

In this way, functions on the spectrum of an operator contain all the information necessary to determine the operator. If the operator in question represents a quantum property, the class of functions must then contain all the quantal information possible about the property.

Our problem consists in extending this connection to an algebra of unbounded operators. Following an idea of Davies [1-2], we consider the following class of functions as suitable.

Recall that in Theorem [5.2] we have constructed a map $\kappa : \mathcal{A}' \to LC(\mathcal{H})$, from $\mathcal{A}'$ into the compact operators on $\mathcal{H}$. We showed there that κ was continuous, injective, and had dense range. As $LC(\mathcal{H})$ is the pre–dual of $\mathcal{L}(\mathcal{H})$, this shows that $\langle \mathcal{L}(\mathcal{H}), \mathcal{A}' \rangle$ forms a dual pair.

The class of functions we are interested in can be expressed in terms of the spectral family of the observable in question. We consider polynomials in the spectral positive operators, and complete this set in the weak topology determined by the dual pairing above. This explains the notation and reasoning behind equation (7.5) below. Let us collect these ideas together as definitions.

7.1 Definition An $\mathcal{A}$-measure is a generalized spectral family B such that there exists a unique $b \in \mathcal{A}_h$ for which the limit

$$\lim_{s\to\infty} \left\| bu - \int_{-s}^{+s} tB(dt)u \right\| = 0 \tag{7.2}$$

holds for all $u \in \mathcal{W}$. The integral is to be an improper $\mathcal{H}$-valued Riemann Stieltjes integral. We indicate the set of $\mathcal{A}$-measures by $\mathcal{M}_+(\mathcal{A})$. For convenience we often abbreviate equation (7.2) by

$$b = \int_{\mathbb{R}} t\, B(dt). \tag{7.3}$$

We say that B represents b, and that b is the resultant of B.

By an $(\mathcal{A}, \mathcal{W})$-measure, or question, we mean an $\mathcal{A}$-measure B such that

$$B(\Delta)\mathcal{W} \subset \mathcal{W}, \qquad \Delta \in \mathrm{Bor}(\mathbb{R}). \tag{7.4}$$

The set of questions is denoted $\mathcal{M}_+(\mathcal{A}, \mathcal{W})$. If B is an $(\mathcal{A}, \mathcal{W})$-measure representing b, we say that B is a question about $b \in \mathcal{A}_h$.

For any $\mathcal{A}$-measure B we define its extent to be the $\sigma(\mathcal{L}(\mathcal{H}), \mathcal{A}')$-closed linear span of $\{B(\Delta) : \Delta \in \mathrm{Bor}(\mathbb{R})\}$:

$$\mathrm{ext}(B) = \sigma(\mathcal{L}(\mathcal{H}), \mathcal{A}') - \mathrm{cl} \bigvee \{B(\Delta) : \Delta \in \mathrm{Bor}(\mathbb{R})\}. \tag{7.5}$$

If B represents $b \in \mathcal{A}_h$, we also write

$$\mathrm{ext}(B) = \mathrm{ext}(b).$$

We introduce a partial order, $\prec$, on $\mathcal{M}_+(\mathcal{A})$ by saying that $B \prec C$ if $\mathrm{ext}(B) \subset \mathrm{ext}(C)$. If $B \prec C$, and B, C represent b, $c \in \mathcal{A}_h$, respectively, we also write $b \prec c$. If $B \prec C$, we say that B has less information than C, or that b has less information than c. ■

It should be noted that equation (7.3) is merely a formal convenience, since for a given $\mathcal{A}$-measure B, the Riemann Stieltjes integral $\int_{\mathbb{R}} t\, B(dt)u$ need not exist for every function $u \in \mathcal{W}$.

In Naimark's spectral theorem [5.16], we showed that the closure $\bar{b}$ of any element $b \in \mathcal{A}_h$ possesses a spectral function B, being the projection to $\mathcal{H}$ of the PVM-valued spectral function E of some self adjoint extension $\tilde{A}$ of $\bar{b} \oplus -\bar{b}$ on $\mathcal{H} \oplus \mathcal{H}$.

It can readily be seen (Akhiezer and Glazman [1]) that

$$\lim_{s \to \infty} \left\| \tilde{A}\xi - \int_{-s}^{s} t\, E(dt)\xi \right\| = 0$$

for all $\xi \in D(\tilde{A})$.

Since $D(\bar{b}) \oplus D(\bar{b}) \subseteq D(\tilde{A})$, and since

$$\langle \eta, B(\Delta)\xi \rangle = \langle \eta \oplus 0, E(\Delta)\xi \oplus 0 \rangle$$

for all $\xi, \eta \in \mathcal{H}$ and all $\Delta \in \mathrm{Bor}\,(\mathbb{R})$, we have

$$\langle \eta, \int_{-s}^{s} t\, B(dt)\xi \rangle = \langle \eta \oplus 0, \int_{-s}^{s} t\, E(dt)(\xi \oplus 0) \rangle$$

for all $\xi, \eta \in \mathcal{H}$ and all $s \geq 0$. Thus

$$\left\| \bar{b}\xi - \int_{-s}^{s} t\, B(dt)\xi \right\| \leq \left\| \tilde{A}(\xi \oplus 0) - \int_{-s}^{s} t\, E(dt)(\xi \oplus 0) \right\|$$

for all $\xi \in D(\bar{b})$, and all $s \geq 0$. Hence

$$\lim_{s \to \infty} \left\| bu - \int_{-s}^{s} t\, B(dt)u \right\| = 0$$

for all $u \in \mathcal{W} \subseteq D(\bar{b})$, showing that the spectral function B is an $\mathcal{A}$-measure representing b.

We conclude that any $b \in \mathcal{A}_h$ is the resultant of at least one $\mathcal{A}$-measure. Indeed, the techniques of Akhiezer and Glazman [1] can be used to show that any spectral function of $\bar{b}$ is an $\mathcal{A}$-measure representing b.

For our purposes, however, we want to know what elements $b \in \mathcal{A}_h$ have questions about them. Any $b \in \mathcal{A}_h$ can be represented by many $\mathcal{A}$-measures, but it may be that b can not be represented by any question. In particular, if $b \in \mathcal{A}_h$ is such that $b : \mathcal{W} \to \mathcal{H}$ is essentially self adjoint, then the spectral function of $\bar{b}$ (which is an $\mathcal{A}$-measure representing b) is most unlikely to be a question, since the operators $\kappa_\Delta(b)$, $(\Delta \in \mathrm{Bor}(\mathbb{R}))$, will most likely not preserve $\mathcal{W}$. This is the case, for example, for the one dimensional position operator. However, it is important to notice that that although the spectral function of a self adjoint operator $\bar{b}$, extending an observable $b \in \mathcal{A}_h$, is uniquely defined, $\mathcal{A}$-measures for b are not uniquely defined in the same way. In general, whether or not a given observable possesses questions about it remains open, and when looking for questions we have to search through the $\mathcal{A}$-measures, and not just the spectral functions.

7.2 Definition An instrument observable is a symmetric operator $b \in \mathcal{A}_h$ for which there exists at least one question $B \in \mathcal{M}_+(\mathcal{A}, \mathcal{W})$ representing it.

An observable $b \in \mathcal{A}_h$ is said to be physically measurable if an instrument observable c exists which has less information than b, so that $c \prec b$.

Finally, an observable b which is not physically measurable is said to be unmeasurable. ■

Clearly, any instrument obervable b is physically measurable. For any question about b, we can construct an instrument (see below) related to the question, and each instrument obtained in this way should be viewed as a way of measuring the observable b. This is in accord with intuition: there exist many ways of measuring a given observable b. We leave the discussion of the completeness and accuracy of such measurements until later.

If $b \in \mathcal{A}_h$ is physically measurable, but is not an instrument observable, any instrument observable $c \in \mathcal{A}_h$ for which $c \prec b$ can be interpreted as defining questions, and hence instuments, which yield partial information about b. Thus we can make measurements which yield approximate information about b, but we cannot measure b directly. If $b \in \mathcal{A}_h$ is unmeasurable, no measurements can be made which yield information about it. It is an open question as to whether or not all observables $b \in \mathcal{A}_h$ are instrument observables, or even whether any unmeasurable observables $b \in \mathcal{A}_h$ exist. We do, however, have a sufficient condition for $b \in \mathcal{A}_h$ to be an instrument observable, and this is good enough to show that observables such as position, momentum and energy are instrument observables. This condition is also sufficient to show that the instrument observables form a dense subset of $\mathcal{A}_h$. Also, we have a fairly weak condition which tells us when an observable $b \in \mathcal{A}_h$ is physically measurable.

We are now in a position to define operations and instruments.

7.3 Definition An operation is a map $Z : \mathrm{Bor}(\mathbb{R}) \to L_+(\mathcal{A})$ satisfying the conditions

$$Z(\emptyset) = 0, \tag{7.6.a}$$

$$Z(\mathbb{R})(\mathbf{1}) = \mathbf{1}, \tag{7.6.b}$$

$$Z(\Delta) \geq 0, \quad \Delta \in \mathrm{Bor}(\mathbb{R}), \tag{7.6.c}$$

$$T\left(Z\left[\bigcup \Delta_j\right](a)\right) = \lim_{n\to\infty} \sum\nolimits_{j\leq n} T(Z[\Delta_j](a)) \tag{7.6.d}$$

for every σ-family $\{\Delta_j : j \in \mathbb{N}\}$, all $a \in \mathcal{A}$, and all $T \in \mathcal{A}'$.

It is also required that there exists an observable $b \in \mathcal{A}_h$ such that

$$\lim_{s\to\infty} \left\| bu - \int_{-s}^{+s} tZ(dt)(\mathbf{1})u \right\| = 0, \qquad u \in \mathcal{W}. \tag{7.7}$$

An instrument is a map $\mathcal{I} : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}\left(\mathcal{A}'[\sigma^*]\right)$ for which there is an operation Z satisfying

$$\mathcal{I} = Z^t. \tag{7.8}$$

Z is the pre-transpose of $\mathcal{I}$. ■

In what follows, we shall not distinguish between the various topologies and their restrictions to the respective real subspaces $\mathcal{A}_h$ and $\mathcal{A}_h{}'$. We shall now formulate the continuity and order properties of these maps. As usual, $L_+(\mathcal{A})$ is the set of positivity preserving linear maps, with no continuity required. However, this is a spurious generality, as such maps are automatically continuous. Similarly, all the elements of $L_+\left(\mathcal{A}'\right)$ are automatically continuous.

It is important for the interpretation of the theory that an instrument define a question, for the resultant of that question is the observable the instrument is testing for. We now prove that such a connection exists.

The converse is a one-many connection. As noted above, this is in accord with intuition: an observable can be measured in many different ways.

7.4 Proposition Given an instrument $\mathcal{I}$, there is a unique question, denoted $M_{\mathcal{I}}(\Delta)$, determined by it. This question is defined by continuous extension from $\mathcal{W}$ to $\mathcal{H}$ of the formula

$$M_{\mathcal{I}}(\Delta)v = Z(\Delta)(\mathbf{1})v, \qquad v \in \mathcal{W}, \tag{7.9}$$

where

$$Z^t = \mathcal{I}. \tag{7.10}$$

Conversely, given any question B, there exist many instruments $\mathcal{I}$ which answer, or measure, B. These all satisfy

$$M_{\mathcal{I}}(\Delta) = B(\Delta). \tag{7.11}$$

By way of example, a continuum of such instruments for measuring B is given by the transposes of the

$$Z_{B,T}(\Delta)(a) = T(a)\, B(\Delta), \tag{7.12}$$

each defined by a state T.

Proof Let $\mathcal{I}$ be an instrument and Z its pre-transpose. From equations (7.6.a-7.6.c) it follows that for each Borel set Δ, $Z(\Delta)$ extends to a bounded operator on $\mathcal{H}$, call it $M_{\mathcal{I}}(\Delta)$. It is obvious that $M_{\mathcal{I}}(\Delta)$ is non-negative and bounded above by $\mathbf{1}$, increasing with Δ, and has the limiting values $M_{\mathcal{I}}(\emptyset) = 0$ and $M_{\mathcal{I}}(\mathbb{R}) = \mathbf{1}$. If we can prove that $M_{\mathcal{I}}$ is σ–additive, it will have been shown to be a generalized spectral family.

Let u, $v \in \mathcal{W}$ be given, and define the map $T_{u,v}$ by

$$[T_{u,v}, a] = \langle u, av\rangle;$$

evidently $T_{u,v} \in \mathcal{A}'$. Using the σ–additivity of Z, we observe that

$$\Delta \to [T_{u,v}, Z(\Delta)\,\mathbf{1}] = \langle u, M_{\mathcal{I}}(\Delta)\, v\rangle$$

is σ–additive. By a result of Thomas [1],

$$\Delta \to M_{\mathcal{I}}(\Delta)\, v$$

is a σ–additive map from $\mathrm{Bor}(\mathbb{R})$ into $\mathcal{H}$ for every $v \in \mathcal{W}$.

We extend this result from $\mathcal{W}$ to $\mathcal{H}$ as follows. With notation as above, let $\xi \in \mathcal{H}$. Using equation (7.6.d) and Thomas [1] again, since

$$\langle M_{\mathcal{I}}(\Delta)\, v, \xi\rangle = \langle v, M_{\mathcal{I}}(\Delta)\, \xi\rangle, \quad \xi \in \mathcal{H}, v \in \mathcal{W}, \Delta \in \mathrm{Bor}(\mathbb{R}),$$

any $\xi \in \mathcal{H}$ defines a σ–additive map

$$\Delta \to M_{\mathcal{I}}(\Delta)\, \xi.$$

Hence $M_{\mathcal{I}}$ is a generalized spectral family.

From its definition as an extension, if we restrict it back to $\mathcal{W}$, we see immediately that $M_{\mathcal{I}}(\Delta)$ is a linear map from $\mathcal{W}$ to itself. Using equation (7.7) for Z to define b, we see that this same equation holds, now with $M_{\mathcal{I}}(dt)$ in place of $Z(dt)\mathbf{1}$. Thus $M_{\mathcal{I}}$ is a question. This is the first half of the proof.

Next, let B be a question and T a state. Consider the map

$$Z_{B,T} : \mathrm{Bor}(\mathbb{R}) \to L_{+}(\mathcal{A})$$

given by equation (7.12) acting on $\mathcal{W}$. Note that $B(\Delta)$ restricted to $\mathcal{W}$ is positive. To see that $Z_{B,T}$ is an operation, observe that conditions (7.6.a) and (7.6.b) are immediate from (7.12)

Let (Δ_j) be a σ–family, let $a \in \mathcal{A}$ and S be a state. Then

$$[S, Z_{B,T}(\Delta)\, a] = T(a)\,[S, B(\Delta)\,|_{\mathcal{W}}].$$

From this we see that it is sufficient to show that

$$[S, B(\Delta)\,|_{\mathcal{W}}]$$

is σ–additive; the extension from states to general functionals is immediate, as $\mathcal{A}'$ is generating.

As S is a state, it has a decomposition into pure states, say,

$$S(a) = \sum\nolimits_k r_k \langle e_k, a e_k \rangle.$$

Now B is strongly σ-additive, so for each k,

$$\Delta \to \langle e_k, B(\Delta)\, e_k \rangle$$

is σ–additive.

Let ν be the counting measure

$$\nu(J) = \sum\nolimits_{k \in J} r_k$$

on $\mathbb{N}$. Consider the function

$$f_n(k) = \langle e_k, B\left(\bigcup\nolimits_{j \le n} \Delta_j\right) e_k \rangle.$$

From the equality

$$\int f_n \, d\nu = \left[S, B\left(\bigcup\nolimits_{j \le n} \Delta_j\right) |_{\mathcal{W}}\right],$$

we see that $f_n \in L^1(\mathbb{N}, d\nu)$.

The sequence (f_n) is monotonically increasing, and we apply the monotone convergence theorem : $f_n \nearrow f$, with

$$f(k) = \langle e_k, B\left(\bigcup_j \Delta_j\right) e_k \rangle$$

and

$$\int f \, d\nu = \left[S, B\left(\bigcup_{j \leq n} \Delta_j\right) |w\right].$$

The normalization condition comes from the normalization of the states, $T(\mathbf{1}) = 1$, and the integrability condition (7.7) comes from equation (7.2) for questions.

Finally, we must show that B may be recovered from M. This is clear from substituting equation (7.12) into equation (7.10) :

$$M_{\mathcal{I}}(\Delta) v = T(\mathbf{1}) B(\Delta) v,$$

and we are done. ■

With the various definitions in hand we are now able to discuss the measuring process again, this time with details. We shall extract the final axiom from this at the end of the chapter.

7.5 Physical Interpretation (1) Let $b \in \mathcal{A}_h$ be a physically measurable observable, and $\mathcal{I}$ an instrument for measuring it. That is, equation (7.9) determines a question $M_{\mathcal{I}}$ from $\mathcal{I}$, and $M_{\mathcal{I}}$ contains less information than some $\mathcal{A}$-measure B representing b:

$$M_{\mathcal{I}} \prec B. \tag{7.13}$$

Suppose the input state is T_{in}, and an individual measurement is made. The probability of obtaining an affirmative reading in the Borel subset Δ of the spectrum of b is

$$\operatorname{prob}(\mathcal{I}; T_{in}; \Delta) = T_{in}\left[M_{\mathcal{I}}(\Delta)\right]. \tag{7.14}$$

Contingent upon obtaining a positive response for Δ, the output, or collapsed state, is

$$T_{out} = \mathcal{I}(\Delta)[T_{in}] \Big/ \mathcal{I}(\Delta)[T_{in}](\mathbf{1}). \tag{7.15}$$

(2) An identical remeasurement performed immediately after the first has the probability of a positive response for the spectral region Δ' of

$$\operatorname{prob}(\mathcal{I}; T_{out}; \Delta') = \operatorname{tr}\left(\frac{\mathcal{I}(\Delta)[T_{in}]\, M_{\mathcal{I}}(\Delta')}{\mathcal{I}(\Delta)[T_{in}]\,(\mathbf{1})}\right). \tag{7.16}$$

This result proves that there is no strict repeatability: if $\Delta' = \Delta$, the probability is not unity!

In view of the importance of this result, we remind the reader where it came from. The algebra and states were chosen so that the basic physical quantities, such as energy, had finite expectation values. An instrument was defined as a linear black box satisfying: states in, states out. The interpretation is essentially the usual one, the simplest generalization of the discrete formula. Finally, the lack of repeatability is obtained simply by applying the same black box twice in a row.

(3) If the first measurement results in a positive response for the region Δ, and the second in a positive response for Δ', the third and final state is

$$T_{final} = \mathcal{I}(\Delta') \circ \mathcal{I}(\Delta)[T_{in}] \Big/ \mathcal{I}(\Delta') \circ \mathcal{I}(\Delta)[T_{in}](\mathbf{1}). \tag{7.17}$$

The lack of repeatability is reinforced by setting $\Delta' = \Delta$ in this formula. Even if a positive response is obtained for the same region Δ in the second individual experiment, the second output state is not the same as the first output state.

Another interesting point is that in the general case, the memory of the input state is not completely eradicated.

(4) For bounded operators, we recover the results of Davies and Lewis. The lack of repeatability, we stress, is due to the continuous spectrum and not the algebra.

Let

$$b = \sum\nolimits_n \beta_n P_n \tag{7.18.a}$$

be an instrument observable with empty essential spectrum. The operation

$$[\mathcal{Z}(\Delta)](a) = \sum \{ P_n a P_n : \beta_n \in \Delta \} \tag{7.18.b}$$

is the formula of von Neumann. This has the well known repeatability, and all the other familiar properties. Thus for such observables we recover the usual results, and ideal instruments exist in such cases. ■

When we measure an observable with an instrument, then there is a certain lack of precision inherent in the results, obviously. We introduce two measures of this imprecision, but this by no means exhausts the possibilities.

7.6 Definition Let $a \in \mathcal{A}_h$ be a physically measurable observable, and $\mathcal{I}$ an instrument to measure it. Then there is an $\mathcal{A}$-measure A whose resultant is a, and a question B, defined by $\mathcal{I}$, such that $B \prec A$. The strong error in measuring a with $\mathcal{I}$ is the function $\mu_{A,B} : \mathrm{Bor}(\mathbb{R}) \times \mathcal{H} \to \mathbb{R}$ given by

$$\mu_{A,B}(\Delta, v) = \|[A(\Delta) - B(\Delta)]v\|$$

for $\Delta \in \mathrm{Bor}(\mathbb{R})$ and $v \in \mathcal{H}$. Clearly

$$0 \leq \mu_{A,B}(\Delta, v) \leq \|v\|.$$

Under the same circumstances, the weak error in measuring a is the function $\sigma_{A,B} : \mathrm{Bor}(\mathbb{R}) \times \mathrm{S} \to [0,1]$ given by

$$\sigma_{A,B}(\Delta, T) = |T[A(\Delta) - B(\Delta)]|$$

for all $T \in \mathrm{S}$ and $\Delta \in \mathrm{Bor}(\mathbb{R})$. We interpret $\sigma_{A,B}(\Delta, T)$ as a measure of the error incurred by measuring a in the state T with the instrument $\mathcal{I}$ when a positive response is obtained for the region Δ. ■

These error bounds are not sensitive to the lack of repeatability. For if $\mathcal{I}$ is an instrument, it defines a question and hence an observable. If the instrument is used to measure the observable it defines, the above functions both identically vanish. Yet the instrument does not generally have the strict repeatability property. Various measures of this can be devised, a task we leave to the interested reader!

7.3 CONTINUITY AND REGULARITY

There are a number of continuity and regularity consequences of the definition of instruments. The proofs are somewhat technical, and we refer the reader to Dubin and Sotelo, [1], for them.

7.7 Proposition (a) An instrument is positivity preserving and σ-additive as a map

$$\mathcal{I} : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}_+ \left(\mathcal{A}'[\mu']\right)_s. \tag{7.19}$$

The subscript s indicates that the space of continuous maps is equipped with the topology of simple convergence.

(b) An instrument $\mathcal{I}$ is inner regular: for all Borel sets Δ,

$$\mathcal{I}(\Delta) = \mathrm{s} - \lim_{K \uparrow \Delta} \mathcal{I}(K), \tag{7.20}$$

where the convergence is in $\mathcal{L}_+ \left(\mathcal{A}'[\mu']\right)_s$, and the limit is with respect to the filtering increasing compact subsets of Δ.

(c) Any instrument is bounded for the topology of simple convergence on $\mathcal{L}\left(\mathcal{A}'[\mu']\right)$.

Proof (a) Since $Z(\Delta) \in \mathcal{L}(\mathcal{A})$ and μ' is a polar topology, $\mathcal{I}(\Delta)$ is an element of $\mathcal{L}(\mathcal{A}'[\mu'])$.

Let T be a positive functional and $a \in \mathcal{K}$ a positive observable. Then $Z(\Delta)a$ is a positive observable, and so

$$\langle \mathcal{I}(\Delta)T, a\rangle = \langle T, Z(\Delta)a\rangle \geq 0,$$

from which it follows that $\mathcal{I}(\Delta)T$ is positive.

With notation as above, let $\Delta_1 \subset \Delta_2$ be real Borel sets. Then

$$\begin{aligned}\langle \mathcal{I}(\Delta_2)T, a\rangle &= \langle T, Z(\Delta_1)a\rangle + \langle T, Z(\Delta_2 - \Delta_1)a\rangle \\ &\geq \langle T, Z(\Delta_1)a\rangle = \langle \mathcal{I}(\Delta_1)T, a\rangle.\end{aligned}$$

It follows that if (Δ_j) is a σ–family, then

$$0 \leq \mathcal{I}\left(\bigcup_{j\leq n}\Delta_j\right)T \leq \mathcal{I}\left(\bigcup_{j\leq n+1}\Delta_j\right)T \leq \mathcal{I}\left(\bigcup_{j}\Delta_j\right)T,$$

showing that the sequence $\left(\mathcal{I}\left(\bigcup_{j\leq n}\Delta_j\right)T\right)_n$ is monotonically increasing in $\mathcal{K}'$ and bounded above.

Since $\mathcal{A}'[\mu']$ is monotone complete, hence σ–monotone complete, there exists a $S \in \mathcal{K}'$ such that

$$\mathcal{I}\left(\bigcup_{j\leq n}\Delta_j\right)T \nearrow S$$

in the μ'–topology. Therefore, for all $a \in \mathcal{A}$,

$$\begin{aligned}S(a) &= \lim_{n\to\infty}\langle \mathcal{I}\left(\bigcup_{j\leq n}\Delta_j\right)T, a\rangle \\ &= \lim_{n\to\infty}\langle T, Z\left(\bigcup_{j\leq n}\Delta_j\right)a\rangle \\ &= \langle T, Z\left(\bigcup_{j}\Delta_j\right)a\rangle \\ &= \langle \mathcal{I}\left(\bigcup_{j}\Delta_j\right)T, a\rangle.\end{aligned}$$

Thus

$$S = \mathcal{I}\left(\bigcup_{j}\Delta_j\right)T,$$

and so

$$\Delta \to \mathcal{I}(\Delta)T$$

is σ–additive for all $T \in \mathcal{K}'$. As $\mathcal{K}'$ is generating, the same holds for all $T \in \mathcal{A}'$.

(b) Recall that any positive Borel measure which is finite on compact subsets of a locally compact Hausdorff space in which every open set is σ–compact is regular (Rudin [1], 2.18). This holds, eg, for $\mathbb{R}$.

Let T be a positive functional and $a \in \mathcal{K}$ a positive observable. Then

$$m : \mathrm{Bor}(\mathbb{R}) \to \mathbb{R}; m(\Delta) = [\mathcal{I}(\Delta)T, a]$$

is a positive measure on $\mathbb{R}$. Now m is bounded,

$$0 \leq m(\Delta) \leq m(\mathbb{R}) < \infty,$$

so it is regular, hence inner regular.

As $\mathbb{R}$ is σ–compact, inner regularity can be written as (Schmüdgen [1])

$$m(\Delta) = \lim_{n\to\infty} m(K_n),$$

where (K_n) is an increasing sequence of compact subsets of Δ,with $K_n \nearrow \Delta$. Using the σ–additivity for instruments proved in part (a),

$$0 \leq [\mathcal{I}(K_n)T, a] \leq [\mathcal{I}(\Delta)T, a].$$

As $\mathcal{A}'[\mu']$ is monotone complete,

$$[\mathcal{I}(\Delta)T, a] = \mu' - \lim_{n\to\infty} [\mathcal{I}(K_n)T, a].$$

This is equation (7.20), and so (b) has been shown.

(c) For any $T \in \mathcal{K}'$,

$$0 \leq \mathcal{I}(\Delta)T \leq \mathcal{I}(\mathbb{R})T$$

shows that $\{\mathcal{I}(\Delta)T : \Delta \in \mathrm{Bor}(\mathbb{R})\}$ is a subset of the order interval $[\![0, \mathcal{I}(\mathbb{R})T]\!]$. As $\mathcal{K}'$ is normal, every order interval is topologically bounded. As $\mathcal{K}'$ is generating, this is true for all functionals $T \in \mathcal{A}'$. ■

Because $\mathcal{W}$ is a nuclear Fréchet space with a countable basis, it is possible to determine the topological properties of the spaces of maps that have appeared. These properties are used in the proofs of the results we are quoting.

7.8 Theorem Given any instrument $\mathcal{I}$,

$$\widehat{\mathcal{I}}(\kappa_\Delta) = \mathcal{I}(\Delta) \tag{7.21.a}$$

extends to define an integral

$$\widehat{\mathcal{I}} : \mathcal{B}_b(\mathbb{R}) \to \mathcal{L}_+\left(\mathcal{A}'[\mu']\right)_s. \tag{7.21.b}$$

That is, $\widehat{\mathcal{I}}$ is a linear map from the bounded Borel functions on $\mathbb{R}$, equipped with the sup norm, which is continuous and positivity preserving. Hence, $\widehat{\mathcal{I}}$ is a bounded Radon measure in the sense of Thomas [2].

Instruments preserve normalization:

$$\mathcal{I}(\mathbb{R})[T](\mathbf{1}) = T(\mathbf{1}), \tag{7.22}$$

for all states T.

Proof The normalization condition (7.22) is immediate from equations (7.6.b) and (7.8).

The first step in constructing an integral formulation is to choose a class of functions analogous to the simple functions of Lebesgue theory. We start from the characteristic functions of all real Borel sets. We shall write $\Sigma(\mathbb{R})$ for the complex linear space these functions generate. For brevity we shall refer to elements of $\Sigma(\mathbb{R})$ as simple functions.

Equation (7.21) determines a well defined map

$$\widehat{\mathcal{I}} : \Sigma(\mathbb{R}) \to \mathcal{L}\left(\mathcal{A}'[\mu']\right)_s.$$

Note that additivity results in the definition of $\widehat{\mathcal{I}}$ being independent of the representation of simple functions by characteristic functions.

We show $\widehat{\mathcal{I}}$ to be continuous. Let $f \in \mathcal{B}_b(\mathbb{R})$ be real valued and nonzero. Choose a representation as a sum of characteristic functions:

$$f = \sum_{i=1}^{n} t_i \kappa_{\Delta(i)}$$

for some disjoint Borel sets $\Delta(i)$ and real numbers t_i. Then

$$\|f\|_\infty = \max |t_i|,$$

so that

$$-\|f\|_\infty \leq f \leq \|f\|_\infty.$$

As $\widehat{\mathcal{I}}$ preserves positivity,

$$-\|f\|_\infty \mathcal{I}(\mathbb{R}) \leq \widehat{\mathcal{I}}(f) \leq \|f\|_\infty \mathcal{I}(\mathbb{R}).$$

This shows that $\widehat{\mathcal{I}}(f)/\|f\|_\infty$ is an element of the order interval $[\![-\mathcal{I}(\mathbb{R}),\mathcal{I}(\mathbb{R})]\!]$ in $\mathcal{L}(\mathcal{A}'[\mu'])$. It follows from this that

$$\left\{\widehat{\mathcal{I}}(f)T/\|f\|_\infty : f \in \Sigma(\mathbb{R})\setminus 0\right\} \subset [\![-\mathcal{I}(\mathbb{R})T,\mathcal{I}(\mathbb{R})T]\!]$$

for any $T \in \mathcal{K}'$.

If p is any continuous seminorm on $\mathcal{A}'[\mu']$, there exists a positive constant C, depending on p and T, such that

$$p\left(\widehat{\mathcal{I}}(f)T\right) \leq C\|f\|_\infty$$

for all real valued functions $f \in \Sigma(\mathbb{R})$. As $\mathcal{K}'$ is generating, this inequality holds for all $T \in \mathcal{A}'$, and by linearity it holds for all functions in $\Sigma(\mathbb{R})$. This proves that $\widehat{\mathcal{I}}$ is continuous.

Now the completion of $\Sigma(\mathbb{R})$ in the sup norm is $\mathcal{B}_b(\mathbb{R})$, the bounded Borel functions. Hence $\widehat{\mathcal{I}}$ extends to

$$\widehat{\mathcal{I}} : \mathcal{B}_b(\mathbb{R}) \to L\left(\mathcal{A}'[\mu']\right)_s.$$

In accordance with general theory, the extension has range in the linear maps, continuous or not. But we shall now show that the range is, in fact, in the continuous maps, $\mathcal{L}(\mathcal{A}'[\mu'])$. To see this, let $f \in \mathcal{B}_b(\mathbb{R})$ be positive valued. For every $n \in \mathbb{N}$, define

$$\Delta_m^n = f^{-1}[\frac{m-1}{n},\frac{m}{n}), \qquad m \in \mathbb{N};$$

this is a real Borel set. As f is bounded, there is an integer M, depending on n, such that

$$\Delta_m^n = \emptyset, \qquad m > M.$$

With this notation, we define the simple function

$$f_n = \sum_{m=1}^{M} \frac{m-1}{n}\kappa_{\Delta_m^n}.$$

This gives an approximating sequence for f, with

$$\|f - f_n\|_\infty \leq n^{-1}.$$

By continuity, $\left(\widehat{\mathcal{I}}(f_n)\right)$ is an approximating sequence for $\widehat{\mathcal{I}}(f)$ in the simple topology on $L\left(\mathcal{A}'[\mu']\right)_s$. Now each $\widehat{\mathcal{I}}(f_n) \in \mathcal{L}_+\left(\mathcal{A}'[\mu']\right)$, and as $\mathcal{A}'[\mu']$ is a Fréchet space, the uniform boundedness condition tells us that $\widehat{\mathcal{I}}(f) \in \mathcal{L}_+\left(\mathcal{A}'[\mu']\right)$.

It remains to show that $\widehat{\mathcal{I}}$ is positive. The approximating sequence (f_n) constructed above has the property that $f_n \nearrow f$ monotonically. Hence,

$$\mathcal{I}(f_n)T \nearrow \mathcal{I}(f)T, \qquad T \in \mathcal{K}'.$$

As $\mathcal{K}'$ is closed, $\mathcal{I}(f)T \in \mathcal{K}'$. This shows positivity for positive functionals. In the usual way, $\mathcal{K}'$ is generating, and this proves the general result. Finally, we note that these properties are precisely those required by Thomas [2] for a vector valued bounded Radon measure. ∎

7.4 COMPOSITION AND CONDITIONING

Suppose a beam, represented by the state T_{in}, is directed onto an instrument $\mathcal{I}_1$. Immediately thereafter, the emerging beam is directed onto a second instrument $\mathcal{I}_2$. Suppose further that a positive result in Δ_1 is obtained from the first individual measurement, and a positive result in Δ_1 from the second. The outcome state is then found as in equation (7.17) ,

$$\mathcal{I}_{1,2}(\Delta_1 \times \Delta_2)[T_{in}] = \mathcal{I}_2(\Delta_2) \circ \mathcal{I}_1(\Delta_1)[T_{in}] \Big/ \mathcal{I}_2(\Delta_2) \circ \mathcal{I}_1(\Delta_1)[T_{in}](\mathbf{1}). \tag{7.23}$$

The map $\mathcal{I}_{1,2}$ has all the properties of an instrument, now generalized to Borel rectangles in $\mathbb{R}^2$. It evidently represents the double measurement process described above. For n such successive measurements, we would get an instrument map from the product sets in $\mathrm{Bor}(\mathbb{R}^n)$. Similarly for operations from $\mathbb{R}^n$.

Examination of equation (7.23) shows that the standard measure theoretic extension from product sets to all of $\mathrm{Bor}\left(\mathbb{R}^2\right)$ leads to a map which is not necessarily the transpose of an operation. It has all the requisite properties, except that its would-be pre-transpose maps elements of $\mathcal{A}$ to elements of its completion, $\mathcal{W}'\widehat{\bigotimes}\mathcal{W}'$.

We present the result on the extension without proof, which goes in the same way as the regularity proofs for one instrument. With the extension defined, we can follow Davies and Lewis in defining the definitions of joint distributions, marginals and conditioning appropriate to our algebra.

7.10 Proposition Let $\mathcal{I}_{1,2}$ be defined on Borel rectangles by equation (7.23) above. Let Z_1 and Z_2 be the corresponding operations; B_1 and B_2 the questions; and b_1 and b_2 the instrument observables.

There exists a unique inner regular Radon measure

$$\mathcal{I}_2 \circ \mathcal{I}_1 : \mathrm{Bor}\left(\mathbb{R}^2\right) \to \mathcal{L}_+\left(\mathcal{A}'[\mu']\right)_s \tag{7.24}$$

extending $\mathcal{I}_{1,2}$ to all of Bor $(\mathbb{R}^2)$. $\mathcal{I}_2 \circ \mathcal{I}_1$ is the transpose of a map

$$Z_1 \circ Z_2 : \text{Bor}\left(\mathbb{R}^2\right) \to L_+\left(\mathcal{W}'\widehat{\bigotimes}\mathcal{W}'\right), \tag{7.25}$$

and is not, in general, an instrument.

We call $\mathcal{I}_2 \circ \mathcal{I}_1$ the composition of $\mathcal{I}_1$ and $\mathcal{I}_2$. The map $Z_1 \circ Z_2$ is known as the joint distribution of Z_2 following Z_1.

The marginal distributions satisfy

$$Z_1 \circ Z_2\,(\mathbb{R} \times \Delta) = Z_1\,(\mathbb{R})\; Z_2\,(\Delta) \tag{7.26.a}$$

and

$$Z_1 \circ Z_2\,(\Delta \times \mathbb{R}) = Z_1\,(\Delta)\; Z_2\,(\mathbb{R}) \tag{7.26.b}$$

Hence

$$Z_1 \circ Z_2\,(\mathbb{R} \times \Delta)\,[1] = Z_1\,(\mathbb{R})\;[B_2\,(\Delta)] \tag{7.27.a}$$

and

$$Z_1 \circ Z_2\,(\Delta \times \mathbb{R})\,[1] = B_1\,(\Delta) \tag{7.27.b}$$

are questions.

The map $\Delta \to Z_1\,(\mathbb{R})\;[B_2\,(\Delta)]$ is known as the question B_2 conditioned by the measurement of B_1 with the instrument $\mathcal{I}_1$. ■

This complication means that we cannot simply compound instruments to an instrument on all the Borel sets of $\mathbb{R}^2$. This is a mathematical, but not a physical, blemish. For a succession of measurements is physically only defined on product Borel sets, one set for each measurement. The above map then suffices for applications. We note that in particular cases, the compounded map can very well be an instrument. The examples presented below have this property.

7.5 A CLASS OF INSTRUMENTS ON $\mathcal{S}\,(\mathbb{R})$

In this section we proceed to find a class of instrument observables which includes the position, momentum and energy observables. For simplicity we restrict ourselves to one dimension, so that $\mathcal{W} = \mathcal{S}\,(\mathbb{R})$, $\mathcal{H} = L^2\,(\mathbb{R})$, and $\mathcal{A} = \mathcal{L}^+\,(\mathcal{S}\,(\mathbb{R}))$ in all that follows.

For an observable b with discrete spectrum, we know that the ideal measurements are associated with the operation

$$a \to \sum \{ P_\lambda a P_\lambda : \lambda \in \Delta \}, \qquad a \in \mathcal{A},\ \Delta \in \mathrm{Bor}(\mathbb{R}), \tag{7.28}$$

where P_λ is the projection operator onto the eigenspace of b corresponding to the eigenvalue λ.

For an observable b with a continuous spectrum, this has the formal generalization

$$a \to \int_\Delta E(s) a E(ds), \qquad a \in \mathcal{A},\ \Delta \in \mathrm{Bor}(\mathbb{R}), \tag{7.29}$$

where E is a PVM-valued spectral function. Although this formula is reasonable for certain operators in Hilbert space, this operator may prove difficult to define for a general $b \in \mathcal{A}_h$, and may not even map elements of $\mathcal{A}$ to $\mathcal{W}'\widehat{\bigotimes}\mathcal{W}'$, let alone $\mathcal{A}$.

Nonetheless we do not want to lose equation (7.29) entirely. In order to do this, we smooth it with a weighting function. We shall choose a translationally invariant form of smoothing. If this is possible, the result is an instrument, and the associated instrument observable is b.

The difficult part is to determine for which class of observables $b \in \mathcal{A}_h$ such a smoothing process works, and to find the largest class of smoothing functions for which the process works for such an instrument observable b. We have found a particular class of instrument observables which includes q, p, and H, and a large class of smoothing functions. Essentially, finding a smoothing function f for an instrument observable $b \in \mathcal{A}_h$ is equivalent to finding a function f such that the operator $f(b)$ belongs to $\mathcal{A}$. In general, this is an open question.

Let $b \in \mathcal{A}_h$ be such that $b : \mathcal{W} \to \mathcal{H}$ is essentially self adjoint, and let $U(\mathbb{R})$ be the strongly continuous one parameter unitary group on $\mathcal{H}$ with infinitesimal generator $\bar{b}$. We shall also suppose that $U_t(\mathcal{W}) \subseteq \mathcal{W}$ for all $t \in \mathbb{R}$, and that the family of maps $\{ U_t|_\mathcal{W} : |t| \leq r \}$ is an equicontinuous subset of $\mathcal{L}(\mathcal{W})$ for any $r > 0$. This implies that $U(\mathbb{R})$ is a locally equicontinuous type C_0 one parameter group on $\mathcal{W}$. It is clear that q and p are observables of this type. Provided the potential is of class Φ, Hunziker's theorem proves that the Hamiltonian is also of this type.

Let E be the PVM-valued spectral function of $\bar{b}$. We shall need the space of functions $f \in \mathcal{W}$ be such that its Fourier transform is of compact support. That is, $g = \mathcal{F}^* f \in \mathcal{D}(\mathbb{R})$. There is no standard notation for this space, and we choose to write $\mathcal{J}$. Functions $f \in \mathcal{J}$ for which $\|f\|_2 = 1$ are of particular importance here. We shall write $\mathcal{J}_1$ for the space of such functions.

Then let $f \in \mathcal{J}_1$. We will show that setting

$$M_b(\Delta) = \int_{\mathbb{R}} \left[|f|^2 * \kappa_\Delta\right](t)\, E(dt)$$
$$= \left[|f|^2 * \kappa_\Delta\right](b), \qquad \Delta \in \mathrm{Bor}(\mathbb{R}), \tag{7.30}$$

defines a question about $b - \alpha\mathbf{1}$, for some constant α, with $\mathrm{ext}(M_b) \prec \mathrm{ext}(E)$.

The operation Z_b corresponding to the question M_b is given by

$$[Z_b(\Delta)](a) = \int_\Delta f_s(b)^* a f_s(b)\, ds, \tag{7.31}$$

for $\Delta \in \mathrm{Bor}(\mathbb{R})$ and $a \in \mathcal{A}$. The operator $f_s(b) \in \mathcal{A}$ is defined by the spectral calculus:

$$f_s(b) = \int_{\mathbb{R}} f(t-s)\, E(dt). \tag{7.32}$$

These instruments were introduced by Davies [1,2] for the operator q, but without the extra constraint of remaining in $\mathcal{L}^+(\mathcal{W})$. It is surprising how difficult it is to prove that these formulas actually do define instruments.

First recall the following families $\left\{ \|\cdot\|_{N;2} : N \geq 0 \right\}$, $\left\{ \|\cdot\|_{N;\infty} : N \geq 0 \right\}$ of norms on $\mathcal{W}$, both of which determine the topology of $\mathcal{W}$:

$$\|u\|_{N;2} = \sup\nolimits_{0 \leq n,m \leq N} \|t^n D^m f\|_2, \qquad u \in \mathcal{W},\ N \geq 0, \tag{7.33.a}$$
$$\|u\|_{N;\infty} = \sup\nolimits_{0 \leq n,m \leq N} \|t^n D^m f\|_\infty, \qquad u \in \mathcal{W},\ N \geq 0. \tag{7.33.b}$$

Let $f \in \mathcal{J}_1$, and use the spectral theorem to find a locally compact separable measure space M, and a finite positive Borel measure (M, μ) on it, a measurable function $X : M \to \mathbb{R}$, and a unitary map

$$V : \mathcal{H} \to L^2(M, d\mu)$$

such that $\xi \in D(\bar{b})$ if and only if $XV\xi \in L^2(M, d\mu)$, and such that

$$V(\bar{b}\xi) = XV\xi, \qquad \xi \in D(\bar{b}). \tag{7.34}$$

We therefore have that

$$[V(U_t\xi)](m) = e^{itX(m)}(V\xi)(m) \tag{7.35}$$

for $\xi \in \mathcal{H}$, $t \in \mathbb{R}$, and $m \in M$.

7.11 Lemma For any $a \in \mathcal{A}$, h_1, $h_2 \in \mathcal{D}(\mathbb{R})$, u, $v \in \mathcal{W}$, the function

$$G(a; h_1, h_2; u, v)(r) = \int_{\mathbb{R}} h_1(r+t)\overline{h_2(t)}\langle v, U_{-t}aU_{r+t}u\rangle\, dt \tag{7.36}$$

belongs to $\mathcal{S}(\mathbb{R})$. Moreover, for any $a \in \mathcal{A}$, h_1, $h_2 \in \mathcal{D}(\mathbb{R})$, m, n, $N \geq 0$, we can find $C > 0$, $M \geq 0$ such that

$$\|G(a; h_1, h_2; u, p^n q^m v)\|_{N;\infty} \leq C\|u\|_{M;2}\|v\|_2 \tag{7.37}$$

for all u, $v \in \mathcal{W}$.

Proof The strong continuity of $U(\mathbb{R})$ and the local equicontinuity of $U(\mathbb{R})|_{\mathcal{W}}$ together imply that the function

$$t \mapsto A(t, r+t; a) = \langle v, U_{-t}aU_{r+t}u\rangle$$

is continuous for any $a \in \mathcal{A}$, u, $v \in \mathcal{W}$, $r \in \mathbb{R}$. Hence the function $G : \mathbb{R} \to \mathbb{C}$ is well defined. Clearly

$$\partial A(t, r+t; a)/\partial r = i\, A(t, r+t; ab)$$

is also well defined.

Now choose a constant L such that

$$\operatorname{supp}(h_1) \cup \operatorname{supp}(h_2) \subseteq [-L, L].$$

We can then find $K > 0$ such that

$$|A(t, s; a)| \leq K, \qquad |s|, |t| \leq L,$$
$$|A(t, s; ab)| \leq K, \qquad |s|, |t| \leq L.$$

It is one step more to show that

$$\left|\partial \left[h_1(r+t)\overline{h_2(t)}A(t, r+t; a)\right] / \partial r\right| \leq K\left(\|h_1\|_\infty + \|h_1'\|_\infty\right)|h_2(t)|$$

for all r, $t \in \mathbb{R}$. We conclude that G is differentiable. Even more, G is infinitely differentiable, and

$$qG(a; h_1, h_2; u, v) = G(a; qh_1, h_2; u, v) - G(a; h_1, qh_2; u, v)$$
$$pG(a; h_1, h_2; u, v) = G(a; ph_1, h_2; u, v) + G(ab; h_1, h_2; u, v).$$

It follows that the lemma will be true if we can prove (7.37) for $N = 0$. To do this, we use the continuity of the unitary group to deduce that if m, n are given, we can find $C > 0$ and $M \geq 0$ such that

$$\|q^m p^n U_{-t}aU_s u\|_2 \leq C\|u\|_{M;2}, \qquad |s|, |t| \leq L.$$

It is then easy to show that

$$\|G(a; h_1, h_2; u, p^n q^m v)\|_\infty \leq C\|h_1\|_\infty \|h_2\|_1 \|u\|_{M;2} \|v\|_2,$$

from which the result follows. ∎

Unless otherwise noted, by f we shall mean a function in $\mathcal{J}_1$, and by g its Fourier transform. For any $s \in \mathbb{R}$, consider $f_s(b) \in \mathcal{L}(\mathcal{H})$ defined by

$$[V(f_s(b)\xi)](m) = f(X(m) - s)\,(V\xi)(m) \tag{7.38}$$

for $\xi \in \mathcal{H}$ and $m \in M$. Clearly

$$\|f_s(b)\| \leq \|f\|_\infty.$$

7.12 Lemma The operator $f_s(b)$ has the following properties:

(i) $$\langle v, f_s(b)u\rangle = (2\pi)^{-1/2} \int_{\mathbb{R}} e^{-ist} g(t) \langle v, U_t u\rangle\, dt, \qquad u, v \in \mathcal{H};$$

(ii) $$f_s(b)|_{\mathcal{W}} \in \mathcal{A};$$

(iii) $$s \mapsto \langle v, f_s(b)^* a f_s(b) u\rangle$$

is an element of $\mathcal{S}(\mathbb{R})$ for all $a \in \mathcal{A}$, u, $v \in \mathcal{W}$.

Proof We content ourselves with outlining the proof. The proof of part (i) consists in substituting the definition of $f_s(b)$ given in (7.38) into the inner product. Then the Fourier transform of f is substituted. The order of integration may be changed by Fubini's theorem, and the result follows.

For m, $n \geq 0$, we can find $C > 0$, $N \geq 0$ such that

$$\|q^m p^n U_t w\|_2 \leq C\, \|w\|_{N;2}$$

for all $t \in \mathrm{supp}(g)$ and $w \in \mathcal{W}$. Thus

$$|\langle p^n q^m v, f_s(b)u\rangle| \leq (2\pi)^{-1/2} C\, \|g\|_1\, \|u\|_{N;2}\, \|v\|_2$$

for all u, $v \in \mathcal{W}$. Then $f_s(b)u \in \mathcal{W}$ for all $u \in \mathcal{W}$. As

$$[f_s(b)|_{\mathcal{W}}]^+ = \overline{f}_s(b),$$

where $\overline{f}$ is the complex conjugate function to f, (ii) is immediate.

By using Fourier transforms and Fubini's theorem as before, it follows that

$$\begin{aligned}\langle v, f_s(b)^* a f_s(b) u\rangle &= (2\pi)^{-1} \int_{\mathbb{R}} e^{-irs} \int_{\mathbb{R}} g(r+t)\overline{g(t)} A(t, r+t; a)\, dt\, dr \\ &= (2\pi)^{-1/2} \left[\mathcal{F}^* G(a; g, g; u, v)\right](s)\end{aligned}$$

for any $s \in \mathbb{R}$, u, $v \in \mathcal{W}$, $a \in \mathcal{A}$, so the result follows. ∎

7.13 Theorem We can define an operation $Z_b : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}_+(\mathcal{A})$ by setting

$$\langle v, [Z_b(\Delta)](a)u\rangle = \int_\Delta \langle v, f_s(b)^* a f_s(b)u\rangle\, ds \tag{7.39}$$

for all $\Delta \in \mathrm{Bor}(\mathbb{R})$, $a \in \mathcal{A}$, and $u, v \in \mathcal{W}$.

Proof For any $a \in \mathcal{A}$, $m, n \geq 0$, we can find $K_1 > 0, N \geq 0$ such that

$$\|\mathcal{F}^* w\|_1 \leq K_1 \|w\|_{N;\infty}, \qquad w \in \mathcal{W}.$$

We can also find $K_2 > 0$, $M \geq 0$ such that

$$\|G(a; g, g; u, p^n q^m v)\|_{N;\infty} \leq K_2 \|u\|_{M;2} \|v\|_2, \qquad u, v \in \mathcal{W}.$$

Then

$$\begin{aligned}\left|\int_\Delta \langle p^n q^m v, f_s(b)^* a f_s(b)u\rangle\right| &\leq (2\pi)^{-1/2} \|\mathcal{F}^* G(a; g, g; u, p^n q^m v)\|_1 \\ &\leq (2\pi)^{-1/2} K_1 K_2 \|u\|_{M;2} \|v\|_2, \qquad u, v \in \mathcal{W}, \Delta \in \mathrm{Bor}(\mathbb{R}).\end{aligned}$$

We deduce that we can find a linear map

$$Z_b(\Delta)(a) : \mathcal{W} \to \mathcal{H}$$

for any $\Delta \in \mathrm{Bor}(\mathbb{R})$ and $a \in \mathcal{A}$, such that for any $m, n \geq 0$ there exist $L > 0$, $M \geq 0$ such that

$$|\langle p^n q^m v, [Z_b(\Delta)](a)u\rangle| \leq L \|u\|_{M;2} \|v\|_2, \qquad u, v \in \mathcal{W}.$$

Then $[Z_b(\Delta)](a) \in \mathcal{L}(\mathcal{W})$ for all $\Delta \in \mathrm{Bor}(\mathbb{R})$ and all $a \in \mathcal{A}$. As

$$[Z_b(\Delta)](a)^+ = [Z_b(\Delta)](a^+),$$

we have that $[Z_b(\Delta)](a) \in \mathcal{A}$ for all $a \in \mathcal{A}$ and $\Delta \in \mathrm{Bor}(\mathbb{R})$. This shows that we have a map $Z_b(\Delta) \in L(\mathcal{A})$ for any $\Delta \in \mathrm{Bor}(\mathbb{R})$.

Now $f_s(b)^* a f_s(b)$ is positive on $\mathcal{W}$ for all s, and so must $[Z_b(\Delta)](a)$ be, for $a \in \mathcal{K}$ and $\Delta \in \mathrm{Bor}(\mathbb{R})$. As

$$L_+(\mathcal{A}) = \mathcal{L}_+(\mathcal{A}),$$

it follows that $Z_b : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}_+(\mathcal{A})$.

It is clear that $Z_b(\emptyset) = 0$, and our usual Fourier transformation method shows that $[Z_b(\mathbb{R})](\mathbf{1}) = \mathbf{1}$.

Let $\{ \Delta_m : m \in \mathbb{N} \}$ be a σ-family in Bor$(\mathbb{R})$, and write Δ for the union of the Δ_m. Now the map

$$\Gamma \mapsto \langle u, [Z_b(\Gamma)]\,(a)u\rangle = \int_\Gamma \langle f_s(b)u, af_s(b)u\rangle\, ds$$

is a finite Borel measure on Bor$(\mathbb{R})$ for any $a \in \mathcal{K}$ and $u \in \mathcal{W}$. It follows that

$$\langle u, [Z_b\,(\Delta)](a)u\rangle = \sum\nolimits_{m\in\mathbb{N}} \langle u, [Z_b(\Delta_m)]\,(a)u\rangle$$

for any $a \in \mathcal{K}$ and $u \in \mathcal{W}$.

If $T \in \mathcal{K}'$, we can find an orthonormal sequence $\{ u_n \}$ in $\mathcal{W}$ and a sequence $\{ r_n \}$ of positive numbers such that

$$T(a) = \sum\nolimits_{n\in\mathbb{N}} r_n \langle u_n, au_n\rangle, \qquad a \in \mathcal{A}.$$

A standard use of the Monotone Convergence Theorem now implies that

$$T([Z_b\,(\Delta)](a)) = \sum\nolimits_{m\in\mathbb{N}} T([Z_b\,(\Delta_m)]\,(a))$$

for all $a \in \mathcal{K}$. Since both $\mathcal{K}$ and $\mathcal{K}'$ are generating, this equation holds for all $a \in \mathcal{A}$ and all functionals $T \in \mathcal{A}'$.

Finally, if $u, v \in \mathcal{W}$, then

$$\langle v, [Z_b\,(\Delta)](1)u\rangle = \int_\Delta \langle f_s(b)v, f_s(b)u\rangle\, ds$$

for all $\Delta \in$ Bor$(\mathbb{R})$. Then

$$\langle v, \int_{-s}^{s} \lambda\,[Z_b\,(d\lambda)]\,(1)u\rangle = \int_M \left[\int_{-s}^{s} \lambda |f(X(m) - \lambda)|^2\, d\lambda\right] \overline{(Vv)(m)}(Vu)(m)\, d\mu(m)$$

for all $u, v \in \mathcal{W}$ and $s \geq 0$. Thus

$$\left[V \int_{-s}^{s} \lambda\,[Z_b\,(d\lambda)]\,(1)u\right](m) = \int_{-s}^{s} \lambda |f(X(m) - \lambda)|^2\, d\lambda (Vu)(m)$$

for $u \in \mathcal{W}$, $s \geq 0$, $m \in M$. Define real constants α, β by

$$\alpha = \int_\mathbb{R} \lambda |f(\lambda)|^2\, d\lambda, \qquad \text{and} \qquad \beta = \int_\mathbb{R} |\lambda|\, |f(\lambda)|^2\, d\lambda.$$

Using

$$\int_\mathbb{R} \lambda |f(X(m) - \lambda)|^2\, d\lambda = X(m) - \alpha$$

for all $m \in M$,

$$\left[V(b-\alpha\mathbf{1})u - V\int_{-s}^{s} \lambda\,[Z_b\,(d\lambda)]\,(\mathbf{1})u\right](m) = \int_{|\lambda|\geq s} \lambda|f(X(m)-\lambda)|^2\,d\lambda(Vu)(m)$$

for all $u \in \mathcal{W}$, $s \geq 0$, $m \in M$.

A straightforward estimate gives

$$\left|\int_{|\lambda|\geq s} \lambda|f(X(m)-\lambda)|^2\,d\lambda(Vu)(m)\right|^2 \leq [|(Vbu)(m)| + \beta|(Vu)(m)|]^2$$

for all $u \in \mathcal{W}$ $s \geq 0$, $m \in M$. We can now deduce that

$$\lim_{s\to\infty}\left\|(b-\alpha\mathbf{1})u - \int_{-s}^{s} \lambda\,[Z_b\,(d\lambda)]\,(\mathbf{1})u\right\| = 0$$

for all $u \in \mathcal{W}$. Hence Z_b is an operation. ∎

We may summarize these results as follows.

7.14 Theorem Let $b \in \mathcal{A}_h$ be such that $b : \mathcal{W} \to \mathcal{H}$ is essentially self adjoint, and suppose that the one parameter unitary group $U(\mathbb{R})$ generated by $\overline{b}$ is such that $\mathcal{W}$ is U-invariant, and that $U(\mathbb{R})\,|_{\mathcal{W}}$ is a locally equicontinuous type C_0 group on $\mathcal{W}$. If $f \in \mathcal{J}_1$, then $Z_b : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}_+(\mathcal{A})$ as defined above is an operation, so defines a question M_b given by

$$[V\,(M_b(\Delta)u)]\,(m) = \int_{\Delta} |f(X(m)-s)|^2\,ds\,(Vu)(m) \tag{7.40.a}$$

with

$$M_b(\Delta) = \left(|f|^2 * \kappa_\Delta\right)(b) \tag{7.40.b}$$

for $u \in \mathcal{H}$, $m \in M$, $\Delta \in \mathrm{Bor}(\mathbb{R})$. Moreover, M_b is a question about $b - \alpha\mathbf{1}$, where

$$\alpha = \int_{\mathbb{R}} \lambda|f(\lambda)|^2\,d\lambda.$$

Since $M_b(\Delta)$ is bounded for all $\Delta \in \mathrm{Bor}(\mathbb{R})$, we have that

$$M_b \prec E,$$

where the $\mathcal{A}$-measure E is the spectral function of $\overline{b}$. ∎

To get a question about b itself, we need merely choose an f such that $\alpha = 0$.

It is worth noting that, in the case of observables such as q, p or H, the local equicontinuity of $U(\mathbb{R})|_{\mathcal{W}}$ is of a special form. If b is one of these observables, then for any $N \geq 0$ we can find a constant $C > 0$ such that for all $t \in \mathbb{R}$ and $w \in \mathcal{W}$,

$$\|U_t w\|_{N;2} \leq C(1 + |t|)^N \|w\|_{N;2}. \tag{7.41}$$

For such operators it turns out to be unnecessary to demand that the Fourier transform of f have compact support. Hence a much larger class of smoothing functions may be used. Notably, f itself may have compact support.

For a general $b \in \mathcal{A}_h$, we could try the following program. Let

$$\tilde{A} : D\left(\tilde{A}\right) \to \mathcal{H} \bigoplus \mathcal{H} \cong L^2\left(\mathbb{R}; \mathbb{C}^2\right)$$

be a self adjoint extension of $\bar{b} \oplus -\bar{b}$. If the strongly continuous one parameter unitary group on $\mathcal{H} \bigoplus \mathcal{H}$ that it generates preserves

$$\mathcal{W} \bigoplus \mathcal{W} \cong \mathcal{S}\left(\mathbb{R}; \mathbb{C}^2\right)$$

and restricts to a locally equicontinuous type C_0 group there, it is easy to extend the above theory to obtain a generalized spectral family

$$F : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}\left(\mathcal{H} \bigoplus \mathcal{H}\right)$$

which preserves $\mathcal{W} \bigoplus \mathcal{W}$ and is such that

$$\lim_{s \to \infty} \left\| \tilde{A} u \oplus v - \int_{-s}^{s} t F(dt)(u \oplus v) \right\| = 0$$

for all $u, v \in \mathcal{W}$. Projecting F onto the first component of $\mathcal{H} \bigoplus \mathcal{H}$, we would obtain a question about b. This approach now gives us a method for finding certain instrument observables $b \in \mathcal{A}_h$ which are not themselves essentially self adjoint.

It is worth noting that questions can provide good approximations to the spectral functions. For simplicity, let us assume that $b \in \mathcal{A}_h$ satisfies the conditions of Theorem [7.14]. If $f \in \mathcal{J}_1$, let us set

$$f_\beta(t) = \beta^{-1} f(t/\beta^2), \qquad \beta > 0;$$

then $f_\beta \in \mathcal{J}_1$.

Let M_β be the question about b associated with f_β. For the rest of this discussion we restrict ourselves to bounded open intervals of $\mathbb{R}$ rather than general Borel sets. We reserve the symbol I for the interval (c, d), and let

$$J = \{ m \in M : |X(m) - c| < \beta \text{ or } |X(m) - d| < \beta \}$$

also have a fixed significance.

We can show that

$$\begin{aligned} &\|[M_\beta(I) - E(I)]\, u\|^2 \\ &\quad \leq \|u\|^2 \int_{|s| \geq 1/\beta} |f(s)|^2 \, ds + \int_J |(Vu)(m)|^2 \, d\mu(m), \end{aligned} \tag{7.42.a}$$

all $u \in \mathcal{H}$ and $\beta > 0$. It follows from this that

$$\lim_{\beta \to 0} \|[M_\beta(I) - E(I)]\, u\| = 0, \qquad u \in \mathcal{H}, \tag{7.42.b}$$

provided neither end point of I is an eigenvalue of b.

Similarly, if $T \in \mathrm{S}$ is an arbitrary state, then decomposing it into pure states enables us to find a positive function $\Phi_T \in L^1(M, d\mu)$ of unit norm, such that

$$\begin{aligned} &|T\,[M_\beta(I) - E(I)]| \\ &\quad \leq \int_{|s| \geq 1/\beta} |f(s)|^2 \, ds + \int_J \Phi_T(m) \, d\mu(m). \end{aligned} \tag{7.43.a}$$

Thus

$$\lim_{\beta \to 0} T\,[M_\beta(I) - E(I)] = 0, \tag{7.43.b}$$

for all bounded open intervals I such that neither end point is an eigenvalue of b.

Hence it is clear that the questions $\{ M_\beta : \beta > 0 \}$ converge to E both strongly and weakly in the sense of Definition (7.6), at least for Borel sets which are bounded open intervals.

Theorem [7.14] has an immediate consequence, which tells us that instrument observables are quite common.

7.15 Theorem The subset of $\mathcal{A}_h$ consisting of instrument observables is sequentially dense in $\mathcal{A}_h$.

Proof Using the notation of Chapter 4, if $b \in \mathcal{A}_h$, then we can find constants $b_{m,n}$, $(m, n \geq 0)$, such that

$$b = \sum_{m,n \geq 0} b_{m,n} u_m \otimes u_n,$$

and we must have

$$\overline{b_{m,n}} = b_{n,m}.$$

If we set

$$b_N = \sum_{m,n \le N} b_{m,n} u_m \otimes u_n,$$

then $b_N \in \mathcal{F} \bigcap \mathcal{A}_h$, and $b_N \to b$ in $\mathcal{A}$ as $N \to \infty$. We shall now prove that b_N is an instrument observable.

First of all, b_N is a bounded self adjoint operator on $\mathcal{H}$, and its one parameter unitary group $U_N(\mathbb{R})$ maps the $N+1$ dimensional subspace, $\mathcal{W}_N$, of $\mathcal{W}$ spanned by $\{w_0, w_1, \ldots, w_N\}$ to itself. On any w_n with $n \geq N+1$, $U_N(\mathbb{R})$ acts as the identity. As the $\{w_n : n \geq 0\}$ is an absolute basis for $\mathcal{W}$, it is clear that $U_N(\mathbb{R})$ maps $\mathcal{W}$ to itself, and restricts to an equicontinuous type C_0 one parameter group in $\mathcal{L}(\mathcal{W})$. We conclude that b_N is an instrument observable. ■

It is possible to relax the requirements of Theorem [7.14] to find a large class of instrument observables. The details of the calculation are straightforward, so we give the result without proof. Let $b \in \mathcal{A}_h$, and write $\sigma_{\mathcal{A}}(b)$ for its spectrum in $\mathcal{A}$. If $z \in \mathbb{C} \setminus \sigma_{\mathcal{A}}(b)$, we let R_z denote the resolvent of b, $(b - z\mathbf{1})^{-1}$, which is an element of $\mathcal{A}$. It is worth noting that the following result does not require that b be essentially self adjoint.

7.16 Theorem If $b \in \mathcal{A}_h$ is such that we can find an $r > 0$ for which

(i)
$$\{ z \in \mathbb{C} : |\Im z| = r \} \bigcap \sigma_{\mathcal{A}}(b) = \emptyset;$$

and for which

(ii)
$$\{ zR_z : |\Im z| = r \} \subseteq \mathcal{A}$$

is an equicontinuous subset of $\mathcal{L}(\mathcal{W})$, then b is an instrument observable. Associated with b is the question

$$[Z_b(\Delta)](a) = (r/\pi) \int_{\Delta} R^{+}_{s+ir} a R_{s+ir}\, ds, \tag{7.44}$$

for $\Delta \in \mathrm{Bor}(\mathbb{R})$ and $a \in \mathcal{A}$. In this case,

$$f(t) = (r/\pi)^{1/2} (t - ir)^{-1}$$

is the appropriate smoothing function. ■

If there exists an r_0 such that the conditions of Theorem [7.16] can be satisfied for all $0 < r < r_0$, then we have a question M_r about b associated with every r in this range. If B is a spectral function for b, it is possible to show that the errors converge as before:

$$\lim_{r\to 0} \|[M_r(I) - B(I)]\,u\| = 0, \qquad u \in \mathcal{H},$$

and

$$\lim_{r\to 0} T\,[M_r(I) - B(I)] = 0, \qquad T \in \mathsf{S}$$

for all bounded open intervals I such that neither end point is an eigenvalue of b.

If $b \in \mathcal{A}_h$ is essentially self adjoint and satisfies the conditions of Theorem [7.14], the standard theory of locally equicontinuous type C_0 one parameter groups on locally convex spaces implies that b also satisfies the conditions of Theorem [7.16]. Thus the class of instrument observables found by Theorem [7.16] is larger than the class found by Theorem [7.14]. On the other hand, [7.16] only finds one weighting function, whereas [7.14] finds many. That is, [7.14] provides many more ways of measuring an observable than does [7.16]. As well, calculating the resolvent R_z is, on the whole, fairly difficult. In summary, then, it is best to check the conditions of Theorem [7.14].

We now know that the set of instrument observables are sequentially dense in $\mathcal{A}_h$, but we have no really easy condition for determining whether or not a given observable is an instrument observable. In contrast, we can now provide a fairly simple test which determines when an observable is simply physically measurable. The condition essentially requires that $\sigma_{\mathcal{A}}(b) \neq \mathbb{C}$.

7.17 Theorem Let $b \in \mathcal{A}_h$ be such that we can find $z \in \mathbb{C} \setminus \mathbb{R}$ with $z \notin \sigma_{\mathcal{A}}(b)$. Then b is physically measurable.

Proof Since

$$(b - z\mathbf{1})^+ = b - \overline{z}\mathbf{1}$$

is invertible if and only if $b - z\mathbf{1}$ is, we may assume that

$$z = x + iy, \qquad x \in \mathbb{R},\ y > 0.$$

Let

$$f(s) = (2\pi y^2)^{-1/2} \exp(-s^2/2y^2).$$

For any $\Delta \in \mathrm{Bor}(\mathbb{R})$, define $Z(\Delta) \in \mathcal{L}(\mathcal{A})$ by the formula

$$Z(\Delta) = \int_\Delta f(s)\,ds\,Q_z[(b - x\mathbf{1})a(b - x\mathbf{1})] + \int_\Delta sf(s)\,ds\,Q_z(ab + ba - 2xa) + \int_\Delta s^2 f(s)\,ds\,Q_z(a), \tag{7.45.a}$$

where

$$Q_z(c) = R_z^+ c R_z \tag{7.45.b}$$

for $a \in \mathcal{A}$.

Then Z is an operation and defines a question M about $2y^2 Q_z(b - x\mathbf{1})$.

Let B be a spectral function for b, obtained by projecting down from the spectral function E for some self adjoint extension $\tilde{A}$ of $\overline{b} \oplus -\overline{b}$ in the usual fashion. For any $\Delta \in \mathrm{Bor}(\mathbb{R})$, if we define the continuous function $G_\Delta : \mathbb{R} \to [0,1]$ by

$$G_\Delta(t) = \left[(t-x)^2 + y^2\right]^{-1} \int_\Delta (t - x + s)^2 f(s)\, ds, \tag{7.46}$$

it is easy to see that

$$\begin{aligned}
\langle v, M(\Delta) u\rangle &= \int_\Delta \langle v, Q_z \left[(b + (s-x)\mathbf{1})^2\right] u\rangle f(s)\, ds \\
&= \int_\Delta \langle v \oplus 0, \left[\tilde{A} + (s-x)\mathbf{1}\right]^2 \left[(\tilde{A} - x\mathbf{1})^2 + y^2\mathbf{1}\right]^{-1} (u \oplus 0)\rangle f(s)\, ds \\
&= \langle v \oplus 0, \int_{\mathbb{R}} G_\Delta(t) E(dt)(u \oplus 0)\rangle \\
&= \langle v \int_{\mathbb{R}} G_\Delta(t) B(dt) u\rangle
\end{aligned}$$

for $u, v \in \mathcal{W}$. Thus

$$M(\Delta) = \int_{\mathbb{R}} G_\Delta(t) B(dt)$$

weakly. From the definition of extent, we can now see that $M(\Delta) \in \mathrm{ext}(B)$ for all $\Delta \in \mathrm{Bor}(\mathbb{R})$, and so $M \prec B$. Thus b is physically measurable. ■

It is worth noting that if we can find $x \in \mathbb{R}$ and $y_0 > 0$ such that $x + iy \notin \sigma_{\mathcal{A}}(b)$ for all $y \geq y_0$, we obtain a sequence of questions, M_y, for all $y \geq y_0$. The associated instrument observables,

$$2y^2 Q_{x+iy}(b - x\mathbf{1})$$

converge strongly to $2(b - x\mathbf{1})$ as $y \to \infty$. On the other hand, the operators $M_y(\Delta)$ do not converge to $B(\Delta)$, either strongly or weakly, in this limit. We conclude that the questions we have introduced in this Theorem do not give very much information about the physically measurable observable b.

Finally, similar arguments to those used in Theorem [7.14] lead to the following result.

7.18 Theorem Let $b_1, b_2 \in \mathcal{A}_h$ be instrument observables which satisfy the conditions of Theorem [7.14], and suppose that $f_1, f_2 \in \mathcal{J}_1$ are appropriate weighting functions, yielding operations we denote by $Z[b_1; f_1]$ and $Z[b_2; f_2]$. Then the composition map $Z[b_1; f_1] \circ Z[b_2; f_2]$, defined in Proposition [7.10], is an operation. For a proof see Sotelo [1] or Dubin and Sotelo [1].

7.6 THE AXIOMS

We have completed our analysis of the measurement process, and can write down the corresponding axiom, number 6. It seems an appropriate place also to gather together the previous axioms. ■

Axiom 1. By an elementary quantum system we mean an assemblage consisting of a fixed finite number N of particles moving nonrelativistically in space $\mathbb{R}^3$ under the influence of their mutual potentials and any external potentials present. These particles are electrons, protons and neutrons or bound aggregates of them. The invariant attributes of such a particle are its mass, charge and spin, and that to a good approximation it may be treated as a point particle. The number $d = 3N$ is known as the number of degrees of freedom of the system. When there is no possible ambiguity, we shall write Σ_d for an elementary quantum system with d degrees of freedom. ■

Axiom 2. Consider an elementary system $\Sigma_{(N,t)}$ consisting of N identical particles of type t, such as electrons, moving in $\mathbb{R}^3$; on physical grounds, the type determines the spin s. By a space of wave functions for the system we shall mean any of the maximal spaces $\mathcal{W}_{(N,t)}[\nu]$ isomorphic to the Schrödinger representation space $\mathcal{S}\left(\mathbb{R}^{3N}\right)_s^{\pm}$, in an obvious notation. The $\pm$ sign is chosen to be $+$ for Bosons and $-$ for Fermions, that is, as $2s+1$ is odd or even. The Hilbert space for the system will then be isomorphic to $L^2\left(\mathbb{R}^{3N}\right)_s^{(\pm)}$. Consider a compound system consisting of N_1 identical particles of type t_1 with spin $s_1, \ldots, N_n$ identical particles of type t_n with spin s_n. Let us write $\mathbf{N}$ for the n-tuple $(N_1, \ldots, N_n)$, and similarly $\mathbf{t}$, $\mathbf{s}$ for the type and spin, respectively. Such a system is indicated by the notation

$$\Sigma_{(\mathbf{N},\mathbf{t})} = \Sigma_{(N_1,t_1)} \bigotimes \cdots \bigotimes \Sigma_{(N_n,t_n)}.$$

The space of wave functions for the compound system is the completed projective tensor product of the subsystem wave function spaces; there are no symmetry constraints between particles of different types. We write

$$\mathcal{W}_{(\mathbf{N},\mathbf{t})} = \widehat{\bigotimes}_{j=1}^{n} \mathcal{W}_{(N_j,t_j)};$$

if no misunderstanding is likely, we shall simply write $\mathcal{W}$. This compound system has

$$3N_1(2s_1+1)+\cdots+3N_n(2s_n+1)$$

degrees of freedom. In all cases the operators compound according to the rules above, and the wave function spaces are nuclear Fréchet spaces. The choice of $\mathcal{W}$ depends firstly on the identification of the coordinate and momentum operators as the generators of the Weyl unitary groups, generalizing the phase space translations of classical mechanics. Secondly, we take it that these same coordinate and momenta operators constitute the basic observables. Combining this with the basic measurement principle that every observable is measurable in every state, we arrive at

$$\mathcal{S}\left(\mathbb{R}^d\right)=\mathcal{C}^\infty\left(q_1,p_1,\ldots,q_d,p_d\right),$$

before including spin and statistics. These are included through the Pauli scheme. ■

Axiom 3. The algebra of observables for the quantum system $\Sigma_{(\vec{N},\vec{t})}$ is the set $\mathcal{L}^+\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$ of adjointable operators in $\mathcal{L}\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$. We equip the algebra $\mathcal{L}^+\left(\mathcal{W}_{(\vec{N},\vec{t})}\right)$ with the topology of bounded convergence inherited from $\mathcal{L}_b\left(\mathcal{W}_{(\vec{N},\vec{t})},\left[\mathcal{W}_{(\vec{N},\vec{t})}\right]_b^{\prime}\right)$ via the antilinear embedding k, and which we denote $\mu_{(\vec{N},\vec{t})}$, or simply μ when the nature of the system is clear. ■

Axiom 4. The space $\mathcal{A}'[\mu']$ of continuous linear functionals on the algebra $\mathcal{A}$ of observables for the quantum system $\Sigma_{(\vec{N},\vec{t})}$ may be identified with $\mathcal{W}[\nu]\widehat{\otimes}\mathcal{W}[\nu]$. It is isomorphic to the set T of $\mathcal{W}$-nuclear operators, the duality with $\mathcal{A}$ being given by the trace. The set $\mathcal{A}'_+$ of $\mathcal{K}$-positive linear functionals is a closed normal generating cone with empty interior. The set S of states consists of the positive functionals satisfying the normalization condition

$$T(\mathbf{1}) = 1.$$

$\mathcal{A}'_+$ may be identified with the positive $\mathcal{W}$-nuclear operators. The states then consist of positive $\mathcal{W}$-nuclear operators satisfying $\operatorname{tr}(\rho) = 1$, known as $\mathcal{W}$-density matrices. $\mathcal{A}'$ is a nuclear Fréchet *–algebra under the operations of multiplying and taking adjoints of density matrices. Hence it is barreled, bornological, Mackey, Montel, reflexive, and separable. It is lmc and Q, but not b*. The density matrix representation affords a decomposition of states into vector states.

The vector states constitute the extreme points of the set of states; hence they are known as pure states. The GNS representation for a pure state is unitarily equivalent to the Schrödinger representation, and is closed, algebraically irreducible, self adjoint, and s–class. ■

Axiom 5. The energy observable for the system is the Hamiltonian operator H, equation (6.6.a). For atomic and molecular systems, the fundamental potential is the underlying Coulomb potential. Considering distances and energies appropriate to such systems, a smoothed Coulomb potential such as equation (6.11.b) may be used. For the limited description of certain phenomena, appropriate empirical potentials may be used, such as wells and barriers. These must be such that $\mathcal{W}$ is stable under the dynamical unitary group

$$U_t = \exp(-itH/\hbar).$$

A sufficient condition for this is that $V \in \Phi$. The dynamical group determines the continuous automorphism groups $\tau(\mathbb{R})$ and $\tau'(\mathbb{R})$ for $\mathcal{A}$ and $\mathcal{A}'$, respectively. The viewpoint wherein the observables remain fixed in time and the states evolve, is known as the Schrödinger picture, $[\![\mathcal{A}, \mathrm{S}, \tau'(\mathbb{R})]\!]$. The equation of motion in this picture is the generalized Schrödinger equation, equation (6.19). An equivalent viewpoint is the Heisenberg picture, $[\![\mathcal{A}, \mathrm{S}, \tau(\mathbb{R})]\!]$, wherein the states remain fixed, and the observables evolve in time. The equation of motion in this picture is equation (6.17). This subsumes Newton's equations as expectation values. If spin and statistics are included, the potential must be symmetrized. ■

Axiom 6. An operation is a countably additive map $Z : \mathrm{Bor}(\mathbb{R}) \to L_+(\mathcal{A})$ which filters upwards from 0 with $Z(\mathbb{R})[\mathbf{1}] = \mathbf{1}$ on $\mathcal{W}$. The Riemann integral $\int tZ(dt)[\mathbf{1}]$ is required to be an element of $\mathcal{A}_h$. An instrument is a map $\mathcal{I} : \mathrm{Bor}(\mathbb{R}) \to \mathcal{L}\left(\mathcal{A}'[\mu']\right)_s$ for which there is an operation Z satisfying $Z^t = \mathcal{I}$. An $\mathcal{A}$-measure is a generalized spectral family B which represents an observable in $\mathcal{A}_h$. A question is an $\mathcal{A}$-measure for which all $B(\Delta) \in \mathcal{L}_+(\mathcal{A})$. An instrument observable is an element of $\mathcal{A}_h$ which can be represented spectrally by a question. An observable can be measured if it has a spectral representation by an $\mathcal{A}$-measure B for which there exists a question C with less information, $C \prec B$. We write $c \prec b$ for the observables they uniquely define. Given an instrument $\mathcal{I}$, there is a unique question $M_{\mathcal{I}}$, and hence a unique observable c, defined by it. c is known as the instrument observable. The instrument is a measuring device for any observable b for which $c \prec b$. Conversely, any question defines many instruments, each of which measures the instrument observable c and any observable with $c \prec b$. For an individual measurement on a state T with an instrument $\mathcal{I}$, the probability of a positive response in the region $\Delta \in \operatorname{Bor}(\mathbb{R})$ is

$$\operatorname{prob}(\mathcal{I}; T_{in}; \Delta) = T_{in}\left[M_{\mathcal{I}}(\Delta)\right].$$

Contingent upon obtaining a positive response for Δ, the output, or collapsed state, is

$$T_{out} = \mathcal{I}(\Delta)\left[T_{in}\right] \Big/ \mathcal{I}(\Delta)\left[T_{in}\right](\mathbf{1}).$$

An identical remeasurement performed immediately after the first will not have a probability of unity for a positive response for the region Δ, in general. Hence there is no strict repeatability. The usual results, including strict repeatability, occur if the observable has no essential spectrum, and if its eigenprojections are observables. ■

Before ending, we ought to note that there are other models of quantum mechanics. In addition to the account found in Jammer [1,2] and references therein, the book of Gudder [1] contains an informative summary of the principal alternative schemes, as well as extensive bibliographies.

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