OBSERVABLES, MAXIMAL SYMMETRIC OPERATORS, POV MEASURES AND THEIR APPLICATIONS IN QUANTUM MECHANICS

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Abstract

Approximate observables, their description in terms of POV measures and the subsequent extension of the orthodox notion of observable are examined. The sense in which the approximate observables are non-ideal observables is considered and a generalised concept of ideal observable is proposed. The conventional requirement of self-adjointness is relaxed to one of maximal symmetry and the PV measures are replaced by the larger set of generalised spectral measures of maximal symmetric operators. The implications for the quantisation problem are discussed and we give some new examples of observables which have no orthodox representation, i.e. observables which can be identified with non-self-adjoint maximal symmetric operators. Particular attention is paid to those aspects of the orthodox theory which rely on specific properties of self-adjoint operators, such as their association with the infinitesimal generators of groups of unitary operators, and we look at the analogous properties in our generalised theory.

I, Robert H Fountain, hereby certify that this thesis has been written by me, that it is the record of my own work, and that it has not been submitted in any previous application for a higher degree.

[redacted]

R H Fountain December 15, 1995

I hereby certify that the candidate has fulfilled the conditions of the Resolution and Regulations appropriate to the degree of Doctor of Philosophy in the University of St Andrews and that he is qualified to submit this thesis in application for that degree.

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K K Wan December 15, 1995

Research Supervisor

I was admitted as a research student under ordinance No. 12 on 1 October 1991, and as a candidate for the degree of Doctor of Philosophy on 1 October 1992.

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Contents

Introduction

Since its introduction into quantum mechanics twenty five years ago, the positive-operator-valued (POV) measure has achieved a cult-like status. Its usefulness as a generalised notion of the orthodox concept of observable, i.e. the projector-valued (PV) measure, is unquestioned. Its significance though remains open to debate.

In the conventional Hilbert space formulation of quantum mechanics, an observable may, by virtue of the spectral theorem, be identified with either a self-adjoint operator or a PV measure. Though this fact is readily pointed out by advocates of the 'PV to POV' generalisation, its implications are often overlooked. While the idempotency and orthogonality properties of the PV measure may not, by themselves, be warranted from a physical viewpoint, there are other, more physically desirable properties of the PV measure which are not possessed by an arbitrary POV measure. These other properties are made clear when one emphasises the role of the PV measure as the spectral measure of a self-adjoint operator. In this context it is possible to maintain the physically desirable properties of the PV measure and yet relax the idempotency and orthogonality requirements. This is clarified in chapter 1 where we reformulate the orthodox description of observable and also the concept of approximate observable in terms of families of probability distribution functions. We show that the statistical unsharpness of approximate observables, which characterises non-ideal measurement, implies a notion of ideal observable which generalises that of orthodox quantum mechanics. As a result, the orthodox theory is extended to include *maximal symmetric operators* as observables. Though all self-adjoint operators are maximal symmetric, the converse is not true, and we give some examples of observables which can be accommodated by our generalised theory but not by the orthodox theory.

The PV measure, or equivalently the spectral measure of a self-adjoint operator, is replaced by the more general spectral measure of a maximal symmetric operator. These *generalised spectral measures* are POV measures. Moreover, there is a one-to-one correspondence between the maximal symmetric operators and the generalised spectral measures of maximal symmetric operators. In particular, the (unique) generalised spectral measure of a self-adjoint operator coincides with its usual spectral measure. Now the PV measures form a proper subset of the generalised spectral measures of maximal symmetric operators, which in turn form a proper subset of the POV measures, and it is our contention that only those POV measures associated with maximal symmetric operators can be regarded as a fundamentally significant generalisation of the orthodox notion of observable.

A paper based on some of the work in chapter 1 has been published recently [1].

Having established maximal symmetric operators as observables, we consider in chapter 2 some situations where an *adapted observable* is more appropriate. An adapted observable, as its name suggests, is simply a modified description of an observable which takes into account certain characteristics of the measurement procedure. The approximate observables, which respect the limited resolution of the measuring device, are obviously adapted observables. Chapter 2 contains some new examples of adapted observables and we highlight some of the subtleties involved in adapting our generalised observables which are absent from the adaption of orthodox observables.

Chapter 3 deals with the question of how to extend the notion of function of a self-adjoint operator to one of function of a maximal symmetric operator. We find that the interpretation of such functions in terms of a rescaling of the measuring device, though valid in the orthodox theory, breaks down in our generalised theory.

Of particular interest in chapter 3 is the relation between maximal symmetric operators and semigroups of isometric operators, which generalises that between self-adjoint operators and groups of unitary operators. The implications of this for maximal symmetric operators in their capacity as Hamiltonian operators are considered.

We conclude with some ideas for prospective developments of the work presented here.

Chapter 1

IDEAL AND NON-IDEAL OBSERVABLES

In this chapter we develop a precise notion of ideal observable in terms of what we shall call maximal families of probability distribution functions, or maximal families for short. Maximal families are regarded as embodying the essential, physically relevant attributes of the family of probability distributions generated by a self-adjoint operator. We are led, quite naturally, to a generalisation of orthodox quantum mechanics where observables need only be represented by maximal symmetric operators, of which the self-adjoint operators are a special case. Some examples are given of observables which can be catered for by our generalised theory but not by the orthodox theory.

Definitions and discussions pertaining to the operator theoretic notions of maximal symmetry, generalised spectral functions, etc. can be found in appendix A.

1.1 Orthodox Observables

In orthodox quantum mechanics an observable A is represented by a self-adjoint operator $\widehat{A}$ defined in an appropriate Hilbert space $\mathcal{H}$. The spectral theorem guarantees a one-to-one correspondence between the set of self-adjoint operators in $\mathcal{H}$ and the set of orthogonal resolutions of the identity (ORIs) on $\mathcal{H}$. The ORI associated with a particular self-adjoint operator $\widehat{A}$ is called the spectral function of $\widehat{A}$ and is denoted $\widehat{E}(\widehat{A};\lambda)$. The spectral decomposition of $\widehat{A}$ is then

$$\widehat{A} = \int_{-\infty}^{\infty} \lambda \, d_\lambda \widehat{E}(\widehat{A};\lambda), \tag{1.1}$$

where the RHS of eqn (1.1) is a strongly convergent Lebesgue-Stieltjes integral.

For a given state, i.e. a unit vector $\phi \in \mathcal{H}$, an observable A generates a unique probability distribution function:

$$F_\phi^A(\lambda) \equiv \langle \phi \mid \widehat{E}(\widehat{A};\lambda)\phi \rangle,$$

so that an observable may be identified with a unique family of probability distribution functions

$$\mathbf{M}^A = \{F_\phi^A : \phi \in \mathcal{H}\}.$$

The probability that upon measurement of A, a value lying in a Borel set $\Delta \in I\!\!R$ is obtained, is assumed to be given by the 'Born formula':

$$F_\phi^A(\Delta) = \langle \phi \mid \widehat{E}(\widehat{A};\Delta)\phi \rangle, \tag{1.2}$$

where $\widehat{E}(\widehat{A};\Delta)$ is a projector-valued (PV) measure called the spectral measure of $\widehat{A}$ and is defined by:

$$\widehat{E}(\widehat{A};\Delta) = \int_\Delta d_\lambda \widehat{E}(\widehat{A};\lambda).$$

The mean and variance of observable A are respectively given by

$$\mathcal{E}(A;\phi) \equiv \int \lambda d_\lambda F_\phi^A(\lambda) \tag{1.3}$$

and

$$\mathcal{V}(A;\phi) \equiv \int \{\lambda - \mathcal{E}(A;\phi)\}^2 \, d_\lambda F_\phi^A(\lambda) = \int \lambda^2 d_\lambda F_\phi^A(\lambda) - \mathcal{E}(A;\phi)^2. \tag{1.4}$$

Now since the domain of $\widehat{A}$ is given by

$$\mathcal{D}(\widehat{A}) = \{\phi : \int_{-\infty}^{\infty} \lambda^2 \, d_\lambda \langle \phi \mid \widehat{E}(\widehat{A};\lambda)\phi \rangle < \infty\},$$

or equivalently

$$\mathcal{D}(\widehat{A}) = \{\phi : \mathcal{V}(A) < \infty\}, \tag{1.5}$$

then $\mathcal{E}(A;\phi)$ and $\mathcal{V}(A;\phi)$ above are physically meaningless unless $\phi \in \mathcal{D}(\widehat{A})$. In this case we have

$$\mathcal{E}(A;\phi) = \langle \phi \mid \widehat{A}\phi \rangle \tag{1.6}$$

and

$$\mathcal{V}(A;\phi) = \left\| \widehat{A}\phi \right\|^2 - \langle \phi \mid \widehat{A}\phi \rangle^2 \tag{1.7}$$

Note that eqn (1.5) is a statement of the physical significance of the domain of a self-adjoint operator. Also note that eqn (1.7) generally cannot be written

$$\mathcal{V}(A;\phi) = \langle \phi \mid \widehat{A}^2\phi \rangle - \langle \phi \mid \widehat{A}\phi \rangle^2$$

as this would require ϕ to be in the domain of $\widehat{A}^2$.

1.2 Generalised Observables

Orthodox observables are usually defined without reference to the experimental procedure used to measure them. Take for example the position observable for a free particle on the real line. This is represented by the self-adjoint operator $\widehat{X}$, where

$$\mathcal{D}(\widehat{X}) = \{\phi \in L^2(\mathbb{R}) : \int_{\mathbb{R}} x^2 |\phi(x)|^2 dx < \infty\}$$

and for $\phi \in \mathcal{D}(\widehat{X})$,

$$\left(\widehat{X}\phi\right)(x) = x\phi(x).$$

The spectral measure of $\widehat{X}$ is

$$\left(\widehat{E}(\widehat{X};\Delta)\phi\right)(x) = \chi_{\Delta}(x)\phi(x),$$

where $\chi_{\Delta}(x)$ is the characteristic function for the set Δ. The probability measure generated by $\widehat{E}(\widehat{X};\Delta)$ is then

$$F_{\phi}^{X}(\Delta) = \int_{\Delta} |\phi(x)|^2 dx.$$

According to the Born formula, $F_{\phi}^{X}(\Delta)$ is the probability of finding the particle in Δ, or, equivalently, the probability that the proposition represented by $\widehat{E}(\widehat{X};\Delta)$ will be found to be true.

A more realistic description would incorporate the limited resolution of the measuring device (MD). Measurements of propositions $\widehat{E}(\widehat{X};\Delta)$ and $\widehat{E}(\widehat{X};\Delta')$ for Δ sufficiently close to Δ' cannot be distinguished in practice. There is a well known procedure for dealing with this, leading to the concept of unsharp or approximate observables. The probability distribution function generated by the spectral function of $\widehat{X}$, i.e.

$$F_{\phi}^{X}(\lambda) = \int_{-\infty}^{\lambda} |\phi(x)|^2 dx$$

is randomised with a probability density function f in the following fashion:

$$F_{\phi}^{X_f}(\lambda) \equiv \int_{-\infty}^{\infty} f(\lambda - \lambda') F_{\phi}^{X}(\lambda')\, d\lambda', \tag{1.8}$$

i.e. $F_{\phi}^{X_f}$ is the convolution of F_{ϕ}^{X} with f. Here the function f is characteristic of a particular MD and it represents the extent of inaccuracy or unsharpness of the nominal value recorded; f is assumed to be symmetric, i.e. $f(\lambda) = f(-\lambda)$, peaked at $\lambda = 0$ and to have a finite variance $\mathcal{V}(f)$. Such an f is referred to as the confidence function of the MD used.

This modified distribution describes non-ideal or unsharp measurements of X. The mean and variance over the new distribution are respectively

$$\mathcal{E}(X_f;\phi) = \mathcal{E}(X;\phi)$$

and

$$\mathcal{V}(X_f;\phi) = \mathcal{V}(X;\phi) + \mathcal{V}(f),$$

so that $F_\phi^{X_f} \neq F_\phi^X$, $\mathcal{E}(X_f;\phi) = \mathcal{E}(X;\phi)$ and $\mathcal{V}(X_f;\phi) > \mathcal{V}(X;\phi)$.

In other words inaccuracy of the measuring device leads to an apparent change in the probability distribution function which results in an increase of the variance. However, the above choice for f means that the average value of the observable is unaffected.

One can formalise this by utilising the notion of approximate observable mentioned earlier. The approximate position observable X_f to the observable X corresponds to a family of probability distribution functions

$$\mathbf{M}^{X_f} = \left\{F_\phi^{X_f} : \phi \in \mathcal{D}(\widehat{X})\right\}$$

generated from $\mathbf{M}^X$ by a confidence function f. Unless f is a delta function, in which case X_f coincides with X, then X_f is an unsharp version of X in the sense that for a given $\phi \in \mathcal{D}(\widehat{X})$ the mean values of X and X_f are the same but the variance of X_f is larger than that of X.

Note that

$$F_\phi^{X_f}(\lambda) = \langle \phi \mid \widehat{F}(\widehat{X}, f; \lambda)\phi\rangle,$$

where

$$\widehat{F}(\widehat{X}, f; \lambda) = \int_{-\infty}^{\infty} d\lambda' f(\lambda - \lambda')\widehat{E}(\widehat{X}; \lambda')$$

and $\widehat{F}(\widehat{X}, f; \lambda)$ is an example of a generalized resolution of the identity (GRI) which extends the notion of an ORI by relaxing the orthogonality and idempotency conditions.

The corresponding generalisation of a PV measure is a positive-operator-valued (POV) measure. GRIs are isomorphic to POV measures in the same way that ORIs are isomorphic to PV measures.

Also note that

$$\widehat{X} = \int_{-\infty}^{\infty} \lambda d_\lambda \widehat{F}(\widehat{X}, f; \lambda), \tag{1.9}$$

and in view of (1.1), $\widehat{F}(\widehat{X}, f; \lambda)$ may be termed an approximate or randomised spectral function of $\widehat{X}$. Clearly the representation (1.9) is not unique; different fs give different randomised spectral functions which correspond to different approximate observables.

This idea can be applied to an arbitrary orthodox observable - in each instance we obtain a randomised distribution with the same mean as the original distribution but with an increased variance.

It is noted that by replacing the PV measure in eqn (1.2) with an arbitrary POV measure a probability interpretation is still valid. This observation is essentially the basis for existing generalised theories of quantum mechanics which permit arbitrary POV measures (or equivalently arbitrary GRIs) to be candidate representations of observables [2, 3, 4, 5, 6, 7].

In the next section the approximate observable concept is turned on its head. Starting with families of PDFs generated by arbitrary GRIs as candidate observables we formulate a notion of ideal observable in terms of 'maximal families of PDFs' and we determine the appropriate (operator) representation of such families.

In the sequel, and in accordance with the orthodox concept of observable, the name 'observable' is generally reserved for ideal observables only, though we may, context permitting, occasionally relax this convention.

1.3 Maximal Symmetric Operators as Observables

Recall from section 1.1 that in the orthodox theory each observable A generates a family $\mathbf{M}^A$ of PDFs, one for each unit vector $\phi \in \mathcal{H}$ through the spectral function $\widehat{E}(\widehat{A};\lambda)$ of the associated self-adjoint operator $\widehat{A}$. In other words $\mathbf{M}^A$ is generated by an orthogonal resolution of the identity or its equivalent PV measure. More generally, a family $\mathbf{M}$ of PDFs is generated by a *generalised* resolution of the identity (GRI) $\widehat{F}(\lambda)$ (appendix B). From now on we shall only consider PDFs generated by GRIs. Note that although a GRI gives rise to a family of PDFs there is no guarantee that any of the PDFs would lead to finite variances. We shall return to this crucial point later.

A natural question arising from all this is whether one can define an observable directly in terms of its association with an appropriate family of PDFs. We shall answer in the affirmative by realising that an observable corresponds to a family of PDFs of values obtained by a certain measurement process which leads to finite expectation values and variances.

Definition 1 *A set* $\mathbf{M} = \{F_\phi : \phi \in \mathcal{H}\}$ *of probability distribution functions* F_ϕ*, one for each unit vector* ϕ *in* $\mathcal{H}$*, is called a family of probability distribution functions on the Hilbert space* $\mathcal{H}$*. If there exists a linear manifold* $\mathcal{D}$ *dense in* $\mathcal{H}$ *such that* $\forall \phi \in \mathcal{D}$*,*

$$\mathcal{E}(F_\phi) \equiv \int \lambda d_\lambda F_\phi(\lambda) < \infty, \quad \mathcal{V}(F_\phi) \equiv \int \{\lambda - \mathcal{E}(F_\phi)\}^2 d_\lambda F_\phi(\lambda) < \infty,$$

then $\mathbf{M}$ *is said to have finite expectation values and variances on* $\mathcal{D}$ *and this is denoted by* $\mathbf{M}(\mathcal{D})$.

As will be obvious presently, families $\mathbf{M}(\mathcal{D}), \mathbf{M}'(\mathcal{D}), \ldots$ of PDFs with the same linear manifold on which they give the same expectation values are related to the same observable. The difference in the variances arises from the imperfections of non-ideal measuring devices. The family $\mathbf{M}(\mathcal{D})$ with the minimum variances corresponds to measurements made with ideal measuring devices.

To formalise this we shall introduce the notion of a maximal family of PDFs on $\mathcal{H}$.

Definition 2 *A family* $\mathbf{M}(\mathcal{D})$ *of probability distribution functions* F_ϕ *on a Hilbert space* $\mathcal{H}$ *is called a maximal family of probability distribution functions on the Hilbert space* $\mathcal{H}$ *if given any other family* $\mathbf{M}'(\mathcal{D})$ *of probability distribution functions* F'_ϕ *on* $\mathcal{H}$ *with the same expectation values on* $\mathcal{D}$*, i.e.*

$$\mathcal{E}(F'_\phi) = \mathcal{E}(F_\phi) \quad \forall \phi \in \mathcal{D},$$

we have either

$$F'_\phi = F_\phi \quad \forall \phi \in \mathcal{D}$$

or

$$\mathcal{V}(F'_\phi) \geq \mathcal{V}(F_\phi) \quad \text{for all } \phi \in \mathcal{D} \quad \text{and} \quad \mathcal{V}(F'_\phi) > \mathcal{V}(F_\phi) \quad \text{for some } \phi \in \mathcal{D}.$$

Note that the notation $\mathbf{M}(\mathcal{D})$ automatically includes the linear manifold $\mathcal{D}$ dense in $\mathcal{H}$ on which expectation values and variances exist.

Lemma 1 *Let* $\widehat{F}'(\lambda)$ *be a GRI for the Hilbert space* $\mathcal{H}$ *which generates a family* $\mathbf{M}(\mathcal{D})$ *of PDFs* $F'_\phi(\lambda)$ *on* $\mathcal{H}$*. Then there exists a symmetric operator* $\widehat{A}'$ *in* $\mathcal{H}$ *with domain* $\mathcal{D}$ *such that*

$$\int \lambda d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle = \langle \phi \mid \widehat{A}'\phi\rangle \quad \forall \phi \in \mathcal{D}$$

and

$$\int \lambda^2 d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle \geq \left\|\widehat{A}'\phi\right\|^2 \quad \forall \phi \in \mathcal{D}.$$

Proof: By a theorem of Naimark [11, p 124], there is an orthogonal resolution of the identity $\widehat{E}_+(\lambda)$ for a Hilbert space $\mathcal{H}_+$ which contains $\mathcal{H}$ as a subspace such that

$$\widehat{F}'(\lambda) = \widehat{P}_+\widehat{E}_+(\lambda)\widehat{P}_+, \quad \text{where } \widehat{P}_+ \text{ is the projector from } \mathcal{H}_+ \text{ onto } \mathcal{H}.$$

We have

$$\int \lambda d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle = \int \lambda d_\lambda \langle \phi \mid \widehat{E}_+(\lambda)\phi\rangle_+ \qquad \forall \phi \in \mathcal{D},$$

where $\langle\cdot\mid\cdot\rangle_+$ signifies scalar product in $\mathcal{H}_+$. Let $\widehat{A}_+$ be the self-adjoint operator in $\mathcal{H}_+$ with $\widehat{E}_+(\lambda)$ as its spectral function. Clearly $\mathcal{D}$ lies in the domain of $\widehat{A}_+$ since

$$\int \lambda^2 d_\lambda \langle \phi \mid \widehat{E}_+(\lambda)\phi\rangle_+ = \int \lambda^2 d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle < \infty \qquad \forall \phi \in \mathcal{D}.$$

It follows that

$$\int \lambda d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle = \langle \phi \mid \widehat{A}_+\phi\rangle_+ = \langle \widehat{P}_+\phi \mid \widehat{A}_+\widehat{P}_+\phi\rangle_+$$

$$= \langle \phi \mid \widehat{P}_+\widehat{A}_+\widehat{P}_+\phi\rangle_+ = \langle \phi \mid \widehat{P}_+\widehat{A}_+\widehat{P}_+\phi\rangle.$$

Introduce the operator $\widehat{A}'$ in $\mathcal{H}$ defined on the domain $\mathcal{D}$ by $\widehat{A}' = \widehat{P}_+\widehat{A}_+\widehat{P}_+$. Then $\widehat{A}'$ is symmetric in $\mathcal{H}$ and satisfies the conditions of the first part of the lemma.

Next we have, on $\mathcal{D}$,

$$\int \lambda^2 d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle = \int \lambda^2 d_\lambda \langle \phi \mid \widehat{E}_+(\lambda)\phi\rangle_+$$

$$= \langle \widehat{A}_+\phi \mid \widehat{A}_+\phi\rangle_+ = \langle \widehat{A}_+\widehat{P}_+\phi \mid \widehat{A}_+\widehat{P}_+\phi\rangle_+$$

$$\geq \langle \widehat{P}_+\widehat{A}_+\widehat{P}_+\phi \mid \widehat{P}_+\widehat{A}_+\widehat{P}_+\phi\rangle_+ = \langle \widehat{A}'\phi \mid \widehat{A}'\phi\rangle$$

$$\Rightarrow \quad \int \lambda^2 d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle \geq \left\|\widehat{A}'\phi\right\|^2.$$

Theorem 1 *Maximal families of probability distribution functions on a Hilbert space $\mathcal{H}$ correspond one-to-one to maximal symmetric operators in $\mathcal{H}$ and that each maximal family of probability distribution functions is generated by the (generalised) spectral function $\widehat{F}(\widehat{A};\lambda)$ of the corresponding maximal symmetric operator $\widehat{A}$ by*

$$F_\phi^{\widehat{A}}(\lambda) \equiv \langle \phi \mid \widehat{F}(\widehat{A};\lambda)\phi\rangle.$$

Proof: First, a maximal symmetric operator is defined to be a symmetric operator which has no proper symmetric extension; a self-adjoint operator is therefore a maximal symmetric operator although the converse is generally false (appendix A).

A family $\mathbf{M}(\mathcal{D})$ of PDFs F_ϕ on $\mathcal{H}$ generated by the (generalised) spectral function $\widehat{F}(\widehat{A};\lambda)$ of a maximal symmetric operator $\widehat{A}$ in $\mathcal{H}$ with domain $\mathcal{D}$ is clearly a maximal family. Since if $\widehat{F}'$ is a GRI which generates a family $\mathbf{M}'(\mathcal{D})$ of PDFs F'_ϕ such that

$\mathcal{E}(F'_\phi) = \mathcal{E}(F_\phi)$ $\forall\phi \in \mathcal{D}$ then, by Lemma 1, there exists a symmetric operator $\widehat{A}'$ with domain $\mathcal{D}$ such that

$$\mathcal{E}(F'_\phi) = \int \lambda d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle = \langle \phi \mid \widehat{A}'\phi\rangle,$$

and since $\langle \phi \mid \widehat{A}\phi\rangle = \mathcal{E}(F_\phi) = \mathcal{E}(F'_\phi) = \langle \phi \mid \widehat{A}'\phi\rangle$, then we have [12, p 130]

$$\widehat{A}'\phi = \widehat{A}\phi \quad \forall\phi \in \mathcal{D}.$$

Also by Lemma 1, we have, on $\mathcal{D}$,

$$\int \lambda^2 d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle \geq \left\|\widehat{A}'\phi\right\|^2 = \left\|\widehat{A}\phi\right\|^2 \quad \Rightarrow \quad \mathcal{V}(F'_\phi) \geq \mathcal{V}(F_\phi).$$

Equality in the above expressions holds only if $\widehat{F}(\widehat{A};\lambda) = \widehat{F}'(\lambda)$. This is because $\widehat{F}'(\lambda)$ would then be a spectral function of $\widehat{A}$, but a maximal symmetric operator possesses a unique spectral function. It follows that the spectral function of a maximal symmetric operator generates a maximal family of PDFs. A related argument applies if the closure of $\widehat{A}$ is maximal symmetric.

Next let $\mathbf{M}'(\mathcal{D})$ be a maximal family of PDFs on $\mathcal{H}$, and let $\widehat{F}'(\lambda)$ be the GRI which generates $\mathbf{M}'(\mathcal{D})$. The associated symmetric operator $\widehat{A}'$ (Lemma 1) possesses at least one spectral function $\widehat{F}''(\lambda)$ which in turn generates a new family $\mathbf{M}''(\mathcal{D})$ of PDFs with $\mathcal{E}(F'_\phi) = \mathcal{E}(F''_\phi)$ on $\mathcal{D}$. We have, by Lemma 1,

$$\int \lambda^2 d_\lambda \langle \phi \mid \widehat{F}'(\lambda)\phi\rangle \geq \left\|\widehat{A}'\phi\right\|^2 = \int \lambda^2 d_\lambda \langle \phi \mid \widehat{F}''(\lambda)\phi\rangle$$

$$\Rightarrow \qquad \mathcal{V}(F'_\phi) \geq \mathcal{V}(F''_\phi).$$

This is a contradiction unless $\widehat{F}'(\lambda) = \widehat{F}''(\lambda)$. It follows that $\widehat{F}'(\lambda)$ has to be a spectral function of $\widehat{A}'$ and moreover, $\widehat{A}'$ cannot admit two distinct spectral functions, i.e. $\widehat{A}'$ is maximal symmetric.

1.3.1 Concept of Observables

Intuitively, an observable is a property of a physical system which can manifest itself quantitatively in the form of numerical values when the system interacts with a certain other system; the other system is the measuring device, the values known as measured values, and the interaction as measuring interaction or process. Generally, even when the system is in a specific state, these numerical values occur in a probabilistic manner. An observable is therefore characterisable by a suitable set of PDFs of these measured values with different PDFs corresponding to different states. Here measuring devices are assumed ideal with perfect resolution. This concept leads us to the following

Mathematical Description of Observables *An observable of a physical system is described uniquely by a maximal family of PDFs on a Hilbert space with the different PDFs corresponding to different states of the system. In other words an observable determines and is determined by a maximal family of PDFs.*

The following result is obtained immediately from the preceding theorem.

Corollary 1 *An observable A defines and is defined by a maximal symmetric operator $\widehat{A}$ with domain $\mathcal{D}$, and the corresponding maximal family $\mathbf{M}(\mathcal{D})$ of PDFs $F_\phi^{\widehat{A}}$ is generated by the spectral function $\widehat{F}(\widehat{A};\lambda)$ of the operator $\widehat{A}$. The resulting expectation values and variances are given respectively in terms of $\widehat{A}$ by*

$$\mathcal{E}(F_\phi^{\widehat{A}}) = \langle \phi \mid \widehat{A}\phi \rangle \quad \textit{and} \quad \mathcal{V}(F_\phi^{\widehat{A}}) = \left\|\widehat{A}\phi\right\|^2 - \mathcal{E}(F_\phi^{\widehat{A}})^2.$$

For brevity we shall simply call $\widehat{A}$ the observable. We have here a generalisation of orthodox quantum mechanics by extending the set of observables beyond the set of self-adjoint operators. It is easy to see that a maximal symmetric operator does resemble a self-adjoint operator in possessing a unique spectral function which serves to generate a unique maximal family of PDFs with expectation values and variances directly calculable using the operators in the same expressions.

We should point out that our generalised notion of observable is far more restrictive than the statement, quite commonly adopted [2, 3, 4], that an observable is defined and identified with a POV measure. We shall argue that such a gross generalisation is untenable. A general POV measure does not generate a maximal family of PDFs. Given an arbitrary GRI $\widehat{F}(\lambda)$ then it may be the case that the set C of states, on which the variances of the PDFs generated by $\widehat{F}(\lambda)$ are finite, is not dense. Indeed there are even GRIs for which C is empty [11, p 132]; this would render the mean values physically meaningless. This situation would arise for example if we allow $\mathcal{V}(f) = \infty$ in the description of approximate observables, corresponding to an infinitely imprecise MD. So, we do not consider an arbitrary POV measure as a description of an observable and we only recognise POV measures associated with maximal symmetric operators as representing observables. We should also mention that it is highly desirable to have a single operator to represent an observable as we have in the form of maximal symmetric operators. This would facilitate, for example, the description of interactions directly involving that observable. In contrast a general POV measure does not correspond to a unique symmetric operator [11, p 131].

If $\widehat{F}(\lambda)$ is a GRI such that a dense set $\mathcal{D}$ exists on which

$$\int_{-\infty}^{\infty} \lambda^2 \, d_\lambda \langle \phi \mid \widehat{F}(\lambda)\phi \rangle < \infty$$

then $\widehat{F}(\lambda)$ defines a symmetric operator $\widehat{S}$ with domain $\mathcal{D}$ by[1]

$$\widehat{S} = \int_{-\infty}^{\infty} \lambda \, d_\lambda \widehat{F}(\lambda).$$

Following Werner [14] we shall call $\widehat{S}$ the expectation operator of $\widehat{F}(\lambda)$. This does not imply that $\widehat{F}(\lambda)$ is necessarily a generalised spectral function of the operator $\widehat{S}$ in the sense of appendix A since we may have

$$\left\|\widehat{S}\phi\right\|^2 \neq \int_{-\infty}^{\infty} \lambda^2 \, d_\lambda \langle \phi \mid \widehat{F}(\lambda)\phi \rangle < \infty.$$

It follows that $\widehat{S}$ is of limited use since not even the variance can be calculated directly from it. As an example consider $\widehat{F}(\widehat{X}, f; \lambda)$, the GRI defined by the approximate observable

[1] It is sometimes claimed that $\widehat{S}$ is self-adjoint ([2, p 36],[6]). Even if $\mathcal{D}$ is chosen to be as large as possible, $\widehat{S}$ need not be self-adjoint or even maximal symmetric. Consider the generalised spectral function $\widehat{F}(\widehat{P}_o(J); \lambda) = \widehat{P}^+ \widehat{E}(\widehat{P}; \lambda)$ from appendix A. We have

$$\mathcal{D}(\widehat{P}_o(J)) = \{\phi : \int_{-\infty}^{\infty} \lambda^2 \, d_\lambda \langle \phi \mid \widehat{F}(\widehat{P}_o(J); \lambda)\phi \rangle < \infty\}$$

and on $\mathcal{D}(\widehat{P}_o(J))$

$$\widehat{P}_o(J) = \int_{-\infty}^{\infty} \lambda \, d_\lambda \widehat{F}(\widehat{P}_o(J); \lambda),$$

where $\widehat{P}_o(J)$ is symmetric but not maximal.

X_f. The expectation operator of $\widehat{F}(\widehat{X}, f; \lambda)$ turns out to be the original operator $\widehat{X}$ which has a unique spectral function which clearly cannot be equal to $\widehat{F}(\widehat{X}, f; \lambda)$; it is clear that the variance cannot be obtained from $\widehat{X}$ without reference to $\widehat{F}(\widehat{X}, f; \lambda)$ (see also [4, pp 146–147]).

Though the finite variance condition is seldom stated explicitly, an exception being [15], numerous authors adopt as generalised observables only those GRIs which have self-adjoint expectation operators [15, 16, 17, 18, 19]. The relevant GRIs invariably arise as randomised ORIs, like the approximate position observable above. Clearly the only GRIs in such a scheme which generate maximal families are the ORIs themselves, i.e. the spectral function of the associated (self-adjoint) expectation operator. This also follows from a result of Kruszyński and de Muynck [15].

1.3.2 The Complex Spectra of Maximal Symmetric Operators

One attribute of self-adjoint operators which is often used as justification for their role as observables is that their spectra consist of real numbers only.

Definition 3 *([21, p 88]) Let $\widehat{A}$ be a closed linear operator defined on a domain $\mathcal{D}(\widehat{A})$, dense in a Hilbert space $\mathcal{H}$, and let λ denote a complex valued parameter. If $(\widehat{A} - \lambda\widehat{I})^{-1}$ exists and is a bounded operator defined everywhere in $\mathcal{H}$, then λ is called a regular point of the operator $\widehat{A}$. All other points of the complex plane comprise the spectrum of $\widehat{A}$, denoted $\sigma(\widehat{A})$.*

Though there are closed non-self-adjoint operators which possess a real spectrum, for the symmetric operators we have the following [22, p 606]:

Theorem 2 *If $\widehat{A}$ is a closed symmetric operator then $\sigma(\widehat{A}) \subseteq \mathbb{R}$ if and only if $\widehat{A}$ is self-adjoint.*

It follows that a non-self-adjoint maximal symmetric operator does not have a purely real spectrum.

In orthodox quantum mechanics, the spectrum of a self-adjoint operator is supposed to contain the possible results of measurement, which in turn are assumed to be real numbers. There has been much discussion about the validity of this assumption [23, pp 34–35],[24, p 58]; however, such matters are of no concern to us for we attach no direct physical significance to the spectrum of a maximal symmetric operator. An observable is first and foremost a maximal family of PDFs - each PDF is defined *on the real line* $\boldsymbol{R}$. Theorem 1 tells us that there is a one-to-one correspondence between maximal families and maximal symmetric operators, thus enabling us to represent an observable by a maximal symmetric operator.

1.3.3 The Role of Symmetric Operators which are Non-Maximal

In view of the popular belief that an arbitrary GRI is a candidate observable, Holevo [25, p 69] has proposed that an arbitrary symmetric operator may represent an observable through its various generalised spectral decompositions. The different generalised spectral functions of a particular symmetric operator are assumed to correspond to different ways of measuring the same observable.

Clearly, within such a scheme an observable is not represented by a symmetric operator alone. It is really a generalised spectral function of a symmetric operator which is being identified with an observable. Furthermore, given a generalised spectral function of a symmetric operator there is no general procedure for recovering the symmetric operator. This is because in general a spectral function of a symmetric operator may also be a spectral function of another symmetric operator. We encounter no such difficulties within our scheme since there is a one-to-one correspondence between the maximal symmetric operators and the generalised spectral functions of maximal symmetric operators.

So what role, if any, should the symmetric operators play in our theory? A symmetric operator, if not maximal, does not determine a unique spectral function and does not by itself represent an observable in our present theory. However a symmetric operator $\widehat{A}_0$

does generate observables in the form of its maximal symmetric extensions.[2] Moreover, $\widehat{A}_0$ can be regarded as the restriction to a particular domain $\mathcal{D}_0 = \mathcal{D}(\widehat{A}_0)$ of observables corresponding to its maximal extensions $\widehat{A}$ in that for states in $\mathcal{D}(\widehat{A}_0)$ we can use the symmetric operator directly to evaluate expectation values and variances, namely we have

$$\mathcal{E}(F_\phi^A) = \langle \phi \mid \widehat{A}_0\phi \rangle, \qquad \mathcal{V}(F_\phi^A) = \left\|\widehat{A}_0\phi\right\|^2 - \langle \phi \mid \widehat{A}_0\phi\rangle^2 \qquad \forall \phi \in \mathcal{D}_0.$$

The different maximal extensions show themselves in different probability distributions since they possess distinct spectral functions.

A further comment on generalised spectral functions is in order here. Not every generalised spectral function of an arbitrary symmetric operator is the generalised spectral function of a maximal symmetric operator. To illustrate this consider the generalised spectral function of the non-maximal symmetric operator $\widehat{P}_o$, as defined in appendix A by

$$\widehat{F}(\widehat{P}_o; \lambda) = \widehat{P}^+ \widehat{E}(\widehat{P}; \lambda).$$

Since we have

$$\mathcal{D}(\widehat{P}_o) = \{\phi : \int_{-\infty}^{\infty} \lambda^2 \, d_\lambda \langle \phi \mid \widehat{F}(\widehat{P}_o; \lambda)\phi\rangle < \infty\}$$

then clearly $\widehat{F}(\widehat{P}_o; \lambda)$ cannot be the generalised spectral function of a maximal symmetric operator $\widehat{M}$ say, since this would imply

$$\mathcal{D}(\widehat{M}) = \mathcal{D}(\widehat{P}_o)$$

and

$$\widehat{P}_o\phi = \int_{-\infty}^{\infty} \lambda \, d_\lambda \, \widehat{F}(\widehat{P}_o; \lambda)\phi = \widehat{M}\phi,$$

i.e. $\widehat{P}_o = \widehat{M}$. Evidently there are GRIs which are permissible observables in Holevo's scheme but not in ours.

1.3.4 Significance or Otherwise of Approximate Observables

The significance or otherwise of approximate observables depends on the nature of the imperfection of measuring devices. Even in the realm of classical physics a measuring

[2] All symmetric operators possess maximal symmetric extensions (appendix A).

device, say a velocity measuring device, would have inherent inaccuracy. The situation is more obvious in classical statistical physics where even the physical systems themselves are realisable only approximately. However, the fundamental issue is not that of the existence of inaccuracy but that of whether the inaccuracy can be arbitrarily reduced. In classical physics one assumes the possibility of arbitrary reduction of inaccuracy in any measurement. It follows that approximate observables, while a useful concept to have in the theory, are not fundamental in classical physics in general. A similar analysis can be used in quantum mechanics. Model theories have been established recently [26] in which the measurement of a quantum observable, *including spin* (cf. [27]), can in principle be reduced to local position measurements by a process of spectral separation, i.e. by channelling various spectral components into spatially disjoint regions, and that this enables a measurement to be achieved with arbitrary accuracy. Hence, in contrast to the inclusion of observables represented by maximal symmetric operators, we regard the inclusion of approximate observables or their associated POV measures as a useful but less fundamental generalisation of orthodox quantum mechanics.

Note that we are considering nonrelativistic quantum mechanics here. Relativistic theory may require separate considerations [28, pp 14–15].

1.4 Some Immediate Applications

To justify the extension of orthodox theory to include maximal symmetric operators we must illustrate what kind of new observables are included and what are the physical and mathematical origin of these new observables. Physically, many of the most important quantum observables originate from classical mechanics. A classical observable is a function $A = A(p, x)$ on the classical phase space Γ_c which is coordinated by the canonical pair (p, x) of momentum and position variables p and x. The quantum counterpart as an operator $\widehat{A}$ in an appropriate Hilbert space is to be established through a process of quantisation. More often than not, even the most sophisticated quantisation schemes such as geometric quantisation fail on at least two counts: first they fail to produce self-adjoint operators, and secondly even when they do they fail to produce a unique self-adjoint operator to correspond to a given classical observable $A = A(p, x)$. We wish, for now, to focus on the lack of self-adjointness on quantization;[3] within the context of orthodox theory one takes the view that these classical observables are not quantisable and hence have no quantum counterpart.

1.4.1 Radial Momentum Operators

Our first example concerns the classical radial momentum p_r in spherical polar coordinates. The canonically quantised p_r is represented by a non-self-adjoint maximal symmetric operator $\widehat{p}_r$ (appendix C, [31, p 89],[32, pp 139–141,157]). Geometric quantisation also fails in this respect [33]. Orthodox theory will therefore not admit a quantum radial momentum observable [34]. The question then arises as to why we should not have a quantum radial momentum observable, especially considering the fact that the classical Hamiltonian in spherical polar coordinates, in which p_r^2 appears, can be quantised to yield a self-adjoint operator. If self-adjointness is insisted upon one can go through a procedure of localisation

[3] Non-uniqueness is not considered to be a serious problem. It merely shows that the quantisation process is incomplete. Uniqueness can be achieved only by considering the physical environment the system is subjected to. See, for example, [29, 30] and section 1.5.

to obtain local radial momentum observables [35]. However, our present generalisation will accept $\widehat{p}_r$ as an observable in its own right. The (generalised) spectral function of $\widehat{p}_r$ in $L^2(\mathbb{R}^3, d\mathbf{r}) \equiv L^2(\mathbb{R}^+, r^2 dr) \otimes L^2(S^2, \sin\theta d\theta d\varphi)$ is shown in Appendix C to be given by

$$\widehat{F}(\widehat{p}_r;\lambda) = \overline{\widehat{F}(\widehat{P}_r;\lambda) \otimes \widehat{I}},$$

where

$$\left(\widehat{F}(\widehat{P}_r;\lambda)\,\phi\right)(r) = \frac{1}{2\pi\hbar\, r}\int_{-\infty}^{\lambda} d\lambda' \int_0^{\infty} dr'\, e^{\not{i}\lambda'(r-r')}\, r'\phi(r'), \qquad \not{i} = \frac{i}{\hbar},$$

from which we can work out the PDFs explicitly.

It is well known that unless $\Delta = \mathbb{R}$, there is no non-trivial solution to the equation

$$\widehat{E}(\widehat{X};\mathbb{R}^+)\widehat{E}(\widehat{P};\Delta)\phi = \phi.$$

It then follows from eqn (1.42) in appendix C and from the unitary equivalence of $\widehat{F}(\widehat{P}_r;\lambda)$ and $\widehat{F}(\widehat{P}_+;\lambda)$ that

$$F_\phi^{\widehat{p}_r}(\Delta) = 1$$

if and only if $\Delta = \mathbb{R}$. In other words there is no state which can be identified with a finite range of radial momentum values. This is to be contrasted with *linear* momentum, or any orthodox observable. The idempotency of the spectral measure $\widehat{E}(\widehat{A};\Delta)$ of a self-adjoint operator $\widehat{A}$, defined in a Hilbert space $\mathcal{H}$, ensures the existence of a state ϕ such that $\widehat{E}(\widehat{A};\Delta)\phi = \phi$, an example being $\phi \equiv (\widehat{E}(\widehat{A};\Delta)\psi)/\left\|\widehat{E}(\widehat{A};\Delta)\psi\right\|$, where ψ is an arbitrary element of $\mathcal{H}$.

Note that this 'unsharpness' of radial momentum has nothing at all to do with imprecise measurement. The operator $\widehat{p}_r$ is maximal symmetric and therefore represents an *ideal* observable in that its (unique) spectral function $\widehat{F}(\widehat{p}_r;\lambda)$ generates a maximal family of PDFs on $L^2(\mathbb{R}^3, d\mathbf{r})$.

1.4.2 Time Operators

There has been much discussion concerning the time-energy uncertainty relation

$$\Delta E \Delta t \geq \frac{\hbar}{2} \tag{1.10}$$

with regard to its validity and interpretation [31, pp 413–414],[37, 38, 39]. It is well known that (1.10) cannot be derived within the formalism of orthodox quantum mechanics in an analogous fashion to its position-momentum counterpart. The reason is that one cannot define a time observable which is canonically conjugate to an energy observable, i.e. there exists no self-adjoint operator $\widehat{T}$ which satisfies, on a certain dense set,

$$\left[\widehat{H}, \widehat{T}\right] = i\hbar \tag{1.11}$$

where $\widehat{H}$ is a positive Hamiltonian operator [39, 40, 41]. Though various schemes exist which will admit self-adjoint time operators [40, 41], they do so only by introducing non-bounded-from-below energy operators and thus give rise to a new problem, namely that of interpreting the negative energies. Our interest lies with the principal objection that (1.10) is devoid of physical meaning on the grounds that there is no self-adjoint operator $\widehat{T}$ that solves eqn (1.11) for a given positive Hamiltonian. One such Hamiltonian is that for a free particle on the real line, which we consider next.

We start with the spectral representation space of the momentum operator $\widehat{P}$ in which $\widehat{P}$ acts like the multiplication operator, i.e.

$$\mathcal{H} = L^2(\mathbb{R}, dp)$$

and

$$\left(\widehat{P}\phi\right)(p) = p\phi(p) \quad \forall \phi \in \mathcal{D}(\widehat{P})$$

where

$$\mathcal{D}(\widehat{P}) = \left\{\phi \in \mathcal{H} : \int_{-\infty}^{\infty} p^2 |\phi(p)|^2 dp < \infty\right\}.$$

The Hamiltonian $\widehat{H}$ is defined by

$$\widehat{H} = \frac{1}{2m}\widehat{P}^2,$$

i.e.

$$\left(\widehat{H}\phi\right)(p) = \frac{p^2}{2m}\phi(p) \quad \forall \phi \in \mathcal{D}(\widehat{H})$$

where

$$\mathcal{D}(\widehat{H}) = \mathcal{D}(\widehat{P}^2) = \left\{\phi \in \mathcal{H} : \int_{-\infty}^{\infty} p^4 |\phi(p)|^2 dp < \infty\right\}.$$

As $\mathcal{H} = L^2(\mathbb{R}^-) \oplus L^2(\mathbb{R}^+)$ then an arbitrary element ϕ of $\mathcal{H}$ can be decomposed thus

$$\phi = \phi_- \oplus \phi_+$$

where

$$\phi_-(p) = \phi(p); \quad p \leq 0,$$

$$\phi_+(p) = \phi(p); \quad p \geq 0.$$

Define the Hilbert space $\widetilde{\mathcal{H}}$ by

$$\widetilde{\mathcal{H}} = L^2(\mathbf{R}^+, dE) \oplus L^2(\mathbf{R}^+, dE)$$

and define a map $\mathcal{U}$ from $\mathcal{H}$ to $\widetilde{\mathcal{H}}$ by

$$\phi = \phi_- \oplus \phi_+ \longrightarrow \widetilde{\phi} = \widetilde{\phi}_- \oplus \widetilde{\phi}_+$$

where

$$\begin{aligned}
\phi_-(p) &\in L^2(\mathbb{R}^-, dp) \\
\phi_+(p) &\in L^2(\mathbb{R}^+, dp) \\
L^2(\mathbb{R}^+, dE) &\ni \widetilde{\phi}_-(E) = \left(\frac{m}{2E}\right)^{\frac{1}{4}} \phi_-(-\sqrt{2mE}) \\
L^2(\mathbb{R}^+, dE) &\ni \widetilde{\phi}_+(E) = \left(\frac{m}{2E}\right)^{\frac{1}{4}} \phi_+(\sqrt{2mE}).
\end{aligned}$$

We have

$$\langle \phi \mid \phi \rangle = \int_{-\infty}^{\infty} |\phi(p)|^2 dp = \int_0^{\infty} |\phi(-p)|^2 dp + \int_0^{\infty} |\phi(p)|^2 dp$$

and as these integrals are over positive values of p then we may make the substitution $p = \sqrt{2mE}$ to obtain

$$\langle \phi \mid \phi \rangle = \int_0^{\infty} |\widetilde{\phi}_-(E)|^2 dE + \int_0^{\infty} |\widetilde{\phi}_+(E)|^2 dE = \langle \widetilde{\phi} \mid \widetilde{\phi} \rangle_{\sim}.$$

The map $\mathcal{U}$ has an inverse $\mathcal{U}^{-1}$, defined by

$$\widetilde{\phi}_-(E) \longrightarrow \phi_-(p) = \left|\frac{p}{m}\right|^{\frac{1}{2}} \widetilde{\phi}_- \left(\frac{p^2}{2m}\right),$$

$$\widetilde{\phi}_+(E) \longrightarrow \phi_+(p) = \left|\frac{p}{m}\right|^{\frac{1}{2}} \widetilde{\phi}_+ \left(\frac{p^2}{2m}\right).$$

Clearly $\mathcal{U}$ is unitary. Let $\widehat{U}$ denote the unitary operator which effects $\mathcal{U}$. Now

$$\widetilde{H} \equiv \widehat{U}\widehat{H}\widehat{U}^{-1} = \widetilde{h} \oplus \widetilde{h}$$

where $\widetilde{h}$ is a self-adjoint operator in $L^2(\mathbb{R}^+, dE)$, defined by

$$\mathcal{D}(\widetilde{h}) = \left\{\phi \in L^2(\mathbb{R}^+, dE) : \int_0^\infty E^2|\phi(E)|^2 dE < \infty\right\}$$

and

$$\left(\widetilde{h}\phi\right)(E) = E\phi(E) \quad \forall \phi \in \mathcal{D}(\widetilde{h}).$$

We have thus obtained the spectral representation of $\widehat{H}$. Next define the operator $\widetilde{t}$ by

$$\mathcal{D}(\widetilde{t}) = \left\{\phi \in L^2(\mathbb{R}^+, dE) : \phi \in AC(\mathbb{R}^+), d\phi/dE \in L^2(\mathbb{R}^+, dE), \phi(0) = 0\right\}$$

and

$$\widetilde{t}\phi = -i\hbar\frac{d\phi}{dE} \quad \forall \phi \in \mathcal{D}(\widetilde{t}).$$

Clearly $\widetilde{t}$ is maximal symmetric with deficiency indices $(1,0)$ (cf. $\widehat{P}_+$ in appendix A). On $\mathcal{D}(\widetilde{h}\widetilde{t}) \cap \mathcal{D}(\widetilde{t}\widetilde{h})$ we have

$$\left[\widetilde{h}, \widetilde{t}\right] = i\hbar,$$

and on $\mathcal{D}(\widetilde{H}\widetilde{T}) \cap \mathcal{D}(\widetilde{T}\widetilde{H})$ the operator $\widetilde{T} \equiv \widetilde{t} \oplus \widetilde{t}$ satisfies

$$\left[\widetilde{H}, \widetilde{T}\right] = i\hbar,$$

where $\widetilde{T}$ is maximal symmetric with deficiency indices $(2,0)$ [42, pp 145,149]. Hence $\widetilde{T}$ is a non-self-adjoint maximal symmetric operator which is canonically conjugate to the (self-adjoint) free particle Hamiltonian $\widetilde{H}$. Transforming back to the original momentum representation, we have

$$\widehat{T} \equiv \widehat{U}^{-1}\widetilde{T}\widehat{U},$$

where $\widehat{T}$ has the formal expression

$$\widehat{T} = -i\hbar\left(\frac{m}{p}\frac{d}{dp} - \frac{1}{2p^2}\right),$$

or, in a more familiar form,

$$\widehat{T} = \frac{1}{2}\left\{\frac{m}{\widehat{P}}\widehat{X} + \widehat{X}\frac{m}{\widehat{P}}\right\} \tag{1.12}$$

where $\widehat{X}$ is the position operator $-i\hbar d/dp$. So eqn (1.12) is just the quantised classical 'time of flight' equation.

Given arbitrary maximal symmetric operators $\widehat{A}$ and $\widehat{B}$ defined in the same Hilbert space, we have, for an arbitrary $\phi \in \mathcal{D}(\widehat{A}) \cap \mathcal{D}(\widehat{B})$, the following,

$$\mathcal{V}(\widehat{A};\phi)\mathcal{V}(\widehat{B};\phi) \geq \frac{1}{4}\left|\langle \widehat{A}\phi \mid \widehat{B}\phi\rangle - \langle \widehat{B}\phi \mid \widehat{A}\phi\rangle\right|^2 .$$

The proof of this statement is identical to that for the case where $\widehat{A}$ and $\widehat{B}$ are self-adjoint [43]. So for $\phi \in \mathcal{D}(\widetilde{H}\widetilde{T}) \cap \mathcal{D}(\widetilde{T}\widetilde{H})$, we have

$$\sqrt{\mathcal{V}(\widetilde{H};\phi)}\sqrt{\mathcal{V}(\widetilde{T};\phi)} \geq \frac{\hbar}{2}.$$

We therefore conclude that in our generalised theory, (1.10) can be given physical meaning insofar as $(\Delta t)^2$ is associated with the variance of a maximal symmetric operator.

1.4.3 Phase Space Distributions

The lack of correspondence between classical observables and self-adjoint operators poses a threat to the validity of those reformulations of orthodox quantum mechanics which inherently rely on quantisation rules. Phase space descriptions of quantum mechanics in terms of pseudo-probability distributions[4] are well known examples [45]. Take the case of the Wigner distribution, which, for a given wave function ϕ, is defined on the classical phase space by

$$W_\phi(p,x) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \phi^*(x+y)\phi(x-y)e^{2ipy}dy.$$

Though it is normalised and possesses the correct momentum and position probability densities as marginals, W_ϕ may take negative values and therefore is not a probability density in the usual sense. Now if $\widehat{A}(\widehat{P},\widehat{X})$ is the quantum counterpart of the classical observable $A(p,x)$, obtained by applying the *Weyl rule* [46] to $A(p,x)$ then

$$\langle \phi \mid \widehat{A}(\widehat{P},\widehat{X})\phi\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(p,x)W_\phi(p,x)dpdx. \tag{1.13}$$

[4]The prefix pseudo signifies that these distributions need not be positive.

In other words the expectation value of the quantum observable $\widehat{A}(\widehat{P}, \widehat{X})$ can be obtained as an average value of a corresponding classical observable over the pseudo-distribution function $W_\phi(p, x)$.

Wan and Sumner [46] have applied the Weyl rule to observables of the form $A(p, x) = x^m p$, where $m > 1$, this yields the symmetric operator

$$\widehat{A} = -i\hbar \left(x^m \frac{d}{dx} + \frac{m}{2} x^{m-1} \right),$$

with an assumed domain $C_o^\infty(\boldsymbol{R})$. They have shown that $\widehat{A}$ possesses self-adjoint extensions if and only if m is even and conclude that, besides the absence of a true, i.e. positive, probability density, the Wigner distribution approach is flawed because of its dependence on a generally invalid quantisation rule. However, within the context of our generalised theory this argument collapses, at least for classical observables like $A(p, x)$ above which can be "quantised" as a symmetric operator, as every symmetric operator possesses at least one maximal symmetric extension.

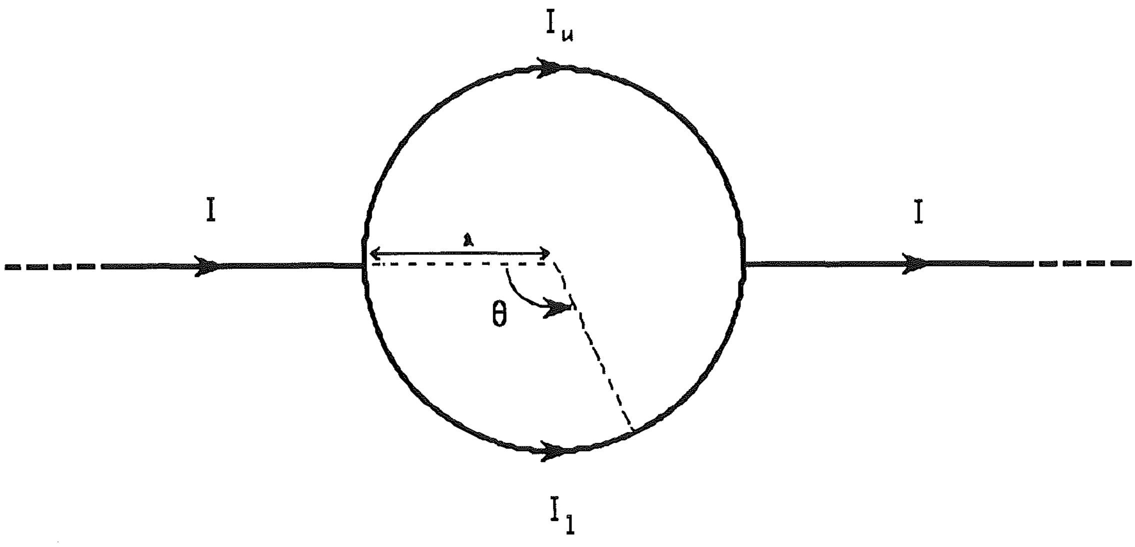

Figure 1.1: A Current-Fed TSCR

1.5 Single-State Macroscopic Quantum Systems

1.5.1 Maximal Symmetric Supercurrent-Operators

We are to consider the system of a thick superconducting ring (TSCR) subject to an applied current which enters the ring at $\theta = 0$ (figure 1.1), passes in parallel through the upper and lower sides of the ring and recombines in the output lead situated at $\theta = \pi$.

Harrison and Wan [47] have studied such a system in detail for the general case where the input and output leads are not necessarily diametrically opposite as in figure 1.1. In their model, a quantum mechanical description of the current through the ring is obtained by associating self-adjoint current operators with the lower and upper paths in the ring. Our aim is to extend Harrison and Wan's analysis by incorporating the input and output leads into the system. We shall see that similarly defined input and output current operators exist though they are represented by non-self-adjoint maximal symmetric operators.

The description in [47] is based on a macroscopic wave function approach to the BCS theory of superconductivity. In the BCS theory, it is assumed that at low temperatures the conduction electrons form pairs, known as Cooper pairs, which behave as bosons and thus they can all occupy the ground state energy level to form a Bose-Einstein condensate. It is the flow of this condensate which gives rise to the supercurrent. A simplified description of this state of affairs is provided by the macroscopic wave function hypothesis whereby the condensate which gives rise to the supercurrent is treated as a single particle of mass $m = 2m_e$ and charge $q = 2e$, where m_e and e are the electronic mass and charge respectively. This quasi-particle can then be described by a single-particle wavefunction [29, 48].

The various current operators associated with the different parts of the system are introduced as follows. Firstly, states of the system 'ring + leads' are assumed to be elements of the Hilbert space

$$\mathcal{H} = \mathcal{H}_{in} \oplus \mathcal{H}_{out} \oplus \mathcal{H}_l \oplus \mathcal{H}_u$$

where

$$\begin{aligned}
\mathcal{H}_{in} &= L^2(\mathbb{R}_{-a}, dx); \quad \mathbb{R}_{-a} = (-\infty, -a], \\
\mathcal{H}_{out} &= L^2(\mathbb{R}_{+a}, dx); \quad \mathbb{R}_{+a} = [a, \infty), \\
\mathcal{H}_l &= L^2(\Theta_l, d\theta); \quad \Theta_l = [0, \pi], \\
\mathcal{H}_u &= L^2(\Theta_u, d\theta); \quad \Theta_u = [\pi, 2\pi].
\end{aligned}$$

However not all elements of $\mathcal{H}$ are permissible states [47], for it is assumed that the wavefunction is single-valued around the ring. Since the points $x = -a$, $\theta = 0$ and $\theta = 2\pi$ are assumed to coincide, as are the points $x = a$ and $\theta = \pi$, then, extending the single valuedness condition to the entire system of ring + leads, we have for $\phi_- \in \mathcal{H}_{in}$, $\phi_+ \in \mathcal{H}_{out}$, $\phi_l \in \mathcal{H}_l$ and $\phi_u \in \mathcal{H}_u$, the following

$$\phi_-(-a) = \phi_l(0) = \phi_u(2\pi) \tag{1.14}$$

and

$$\phi_+(a) = \phi_l(\pi) = \phi_u(\pi). \tag{1.15}$$

The possible momentum operators in $\mathcal{H}_l$ form a one parameter family

$$\{\widehat{P}_{\varphi_l} : \varphi_l \in (-\pi, \pi]\},$$

where

$$\mathcal{D}(\widehat{P}_{\varphi_l}) = \left\{\phi^l \in \mathcal{H}_l : \phi^l \in AC(\Theta_l), d\phi^l/d\theta \in \mathcal{H}_l, \phi^l(0) = e^{-i\varphi_l}\phi^l(\pi)\right\}$$

and

$$\widehat{P}_{\varphi_l}\phi^l = -\frac{i\hbar}{a}\frac{d\phi^l}{d\theta} \qquad \forall \phi^l \in \mathcal{D}(\widehat{P}_{\varphi_l}).$$

The eigenfunctions of $\widehat{P}_{\varphi_l}$ are

$$\psi^l_{\varphi_l,n_l}(\theta) = \frac{1}{\sqrt{2\pi a}} \exp i\,(2\pi n_l + \varphi_l)\,\frac{\theta}{\pi}; \quad n_l = 0, \pm 1, \pm 2, \ldots$$

with corresponding eigenvalues

$$P_{\varphi_l,n_l} = (2\pi n_l + \varphi_l)\,\frac{\hbar}{a\pi}.$$

Likewise the possible momentum operators in $\mathcal{H}_u$ form a one parameter family

$$\{\widehat{P}_{\varphi_u} : \varphi_u \in (-\pi, \pi]\},$$

where

$$\mathcal{D}(\widehat{P}_{\varphi_u}) = \left\{\phi^u \in \mathcal{H}_u : \phi^u \in AC(\Theta_u), d\phi^u/d\theta \in \mathcal{H}_u, \phi^u(\pi) = e^{i\varphi_u}\phi^u(2\pi)\right\}$$

and

$$\widehat{P}_{\varphi_u}\phi^u = -\frac{i\hbar}{a}\frac{d\phi^u}{d\theta} \qquad \forall \phi^u \in \mathcal{D}(\widehat{P}_{\varphi_u}).$$

The eigenfunctions of $\widehat{P}_{\varphi_u}$ are

$$\psi^u_{\varphi_u,n_u}(\theta) = \frac{1}{\sqrt{2\pi a}} \exp i\,(2\pi n_u + \varphi_u)\,\frac{(2\pi - \theta)}{\pi}; \quad n_u = 0, \pm 1, \pm 2, \ldots$$

with corresponding eigenvalues

$$P_{\varphi_u,n_u} = (2\pi n_u + \varphi_u)\,\frac{\hbar}{a\pi}.$$

Note that for arbitrary $\varphi_l, n_l, \varphi_u, n_u$ we have

$$\psi^l_{\varphi_l n_l}(0) = \psi^u_{\varphi_u n_u}(2\pi)$$

and, provided $\varphi_u = \varphi_l$, then

$$\psi^l_{\varphi_l n_l}(\pi) = \psi^u_{\varphi_u n_u}(\pi).$$

So there exist $\psi^l_{\varphi_l n_l}$ and $\psi^u_{\varphi_u n_u}$ which are consistent with the requirement of single valuedness of the wavefunction.

The pre-quantized current in [47] for the lower path is assumed to be

$$j = 2eJ_p \tag{1.16}$$

where J_p is the probability current, which, for a given wave function $\phi^l \in \mathcal{H}_l$, is defined by

$$J_p = -\frac{i\hbar}{2m}\left(\phi^{l*}\frac{\partial \phi^l}{\partial x} - \phi^l \frac{\partial {\phi^l}^*}{\partial x}\right). \tag{1.17}$$

Substituting $\phi^l = \psi^l_{\varphi_l,n_l}$ into (1.16) via (1.17) yields

$$j = \left(\frac{e}{\pi a m}\right) P_{\varphi_l,n_l} \equiv j_{\varphi_l,n_l}.$$

In view of this, the current-operator associated with the lower path is taken to be

$$\widehat{J}_{\varphi_l} = \left(\frac{e}{\pi a m}\right) \widehat{P}_{\varphi_l}$$

where $\widehat{J}_{\varphi_l}$ and $\widehat{P}_{\varphi_l}$ share a common set of eigenfunctions $\{\psi^l_{\varphi_l,n_l} : n_u = 0, \pm 1, \pm 2, \ldots\}$. A current-operator for the upper path is defined similarly.

As we remarked earlier, in [47] the supercurrent fed into the ring is fixed and treated as an external parameter. Suppose this supercurrent has magnitude I. By symmetry, the current will split equally into the lower and upper paths as current magnitudes I_l and I_u, i.e. $I_l = I_u = I/2$. For superconductivity to be maintained we assume I_l and I_u are below the critical current for the ring, I_c^R, i.e. $I < 2I_c^R$. By equating I_l with the eigenvalues j_{φ_l,n_l} of $\widehat{J}_{\varphi_l}$ we can express φ_l and n_l in terms of I:

$$I = j_{\varphi_l,n_l} = \frac{e\hbar}{\pi^2 a^2 m}(2\pi n_l + \varphi_l)$$

or

$$n_l + \frac{\varphi_l}{2\pi} = \frac{\pi a^2 m}{2e\hbar} I. \tag{1.18}$$

Now since n_l is an integer and $-\pi < \varphi_l \leq \pi$ then (1.18) determines unique values for both n_l and φ_l. Likewise n_u and φ_u are uniquely determined by the input current. Clearly we have $n \equiv n_l = n_u$ and $\varphi \equiv \varphi_l = \varphi_u$. The eigenfunctions $\psi^l_{\varphi_l,n_l}$ and $\psi^u_{\varphi_u,n_u}$ may thus be relabelled as ψ^l_I and ψ^u_I.

We now wish to introduce supercurrent operators for the leads in a similar way in order to give quantum mechanical meaning to the input/output current I.

There is a unique choice for the 'input momentum' operator (see next section), this is the non-self-adjoint maximal symmetric operator $\widehat{P}_{in}$ defined on

$$\mathcal{D}(\widehat{P}_{in}) = \{\phi \in \mathcal{H}_{in} : \phi \in AC(\mathbb{R}_{-a}), d\phi/dx \in \mathcal{H}_{in}, \phi(-a) = 0\}$$

by

$$\widehat{P}_{in}\phi = -i\hbar\frac{d\phi}{dx}.$$

Now $\widehat{P}_{in}$ possesses formal eigenfunctions $\phi_k = (1/\sqrt{2\pi})exp(ikx)$, $k \in \mathbb{R}$, with corresponding eigenvalues $\hbar k$, though these are not generalised eigenfunctions in the usual sense since they are not orthogonal [25, p 63] and are not locally in the domain of $\widehat{P}_{in}$ - they do not vanish at $x = -a$.

Evaluating $2eJ_p$, where J_p is the probability current defined by $J_p = (-i\hbar/2m)(\phi^*_{in}\partial\phi_{in}/\partial x - \phi_{in}\partial\phi_{in}{}^*/\partial x)$, for $\phi_{in} = \phi_k$ yields $j_k = (e/\pi m)\hbar k$ and so the current operator associated with the input lead is taken to be

$$\widehat{J}_{in} = \frac{e}{\pi m}\widehat{P}_{in}.$$

Clearly $\widehat{J}_{in}$ is maximal symmetric but not self-adjoint.

An output-current operator, $\widehat{J}_{out}$, can be introduced in an analogous fashion.

Notice that for $\phi_l = \psi^l_I$ and $\phi_u = \psi^u_I$, the single valuedness condition (1.14) cannot be satisfied for any $\phi_- \in \mathcal{D}(\widehat{J}_{in})$ since in this case $\phi_l(0) = \phi_u(2\pi) \neq 0$ whereas $\phi_-(-a) = 0$. However, as we shall see, the quantisation process is not yet complete. In section 1.5.3 we obtain a supercurrent-operator for the entire system by appropriately summing up the supercurrent-operators for the leads and ring. As a result, this incompatibility is removed.

1.5.2 Josephson's Equation

Here we present a novel derivation of Josephson's Nobel prize-winning result that the supercurrent which tunnels through a thin (typically 10Å) insulating barrier separating two superconductors has a sinusoidal dependence on the phase difference in the wave function across the barrier. This is to be contrasted with Feynman's derivation [49], an abridged version of which is given in appendix D.

The two superconductors are assumed to occupy the intervals $\mathbb{R}_o^- \equiv (-\infty, 0)$ and $\mathbb{R}_o^+ \equiv (0, \infty)$, with the insulating barrier, or Josephson junction (hereafter abbreviated to JJ), located at the origin.

Adopting the macroscopic wavefunction approach as in section 1.5.1 above, we shall first of all seek appropriate supercurrent and Hamiltonian operators for this system.

Supercurrent Operators

We start with the operator $\widehat{P}_-^o$ defined in $\mathcal{H}_- \equiv L^2(\mathbb{R}_o^-)$ by

$$\mathcal{D}(\widehat{P}_-^o) = C_o^\infty(\mathbb{R}_o^-)$$

and

$$\widehat{P}_-^o \phi = -i\hbar \frac{d\phi}{dx} \quad \forall \phi \in \mathcal{D}(\widehat{P}_-^o),$$

where $C_o^\infty(\mathbb{R}_o^-)$ is the set of infinitely differentiable functions of compact support in $\mathbb{R}_o^-$. Now $\widehat{P}_-^o$ is symmetric and has adjoint $(\widehat{P}_-^o)^\dagger$ defined on [58, p 160]

$$\mathcal{D}\left((\widehat{P}_-^o)^\dagger\right) = \{\phi_- \in \mathcal{H}_- : \phi_- \in AC(\mathbb{R}_o^-), d\phi_-/dx \in \mathcal{H}_-\}$$

by

$$(\widehat{P}_-^o)^\dagger \phi_- = -i\hbar \frac{d\phi_-}{dx}.$$

Proposition: *The operator $\widehat{P}_-^o$ has a unique maximal symmetric extension, this being its closure $\overline{\widehat{P}_-^o}$.*

Proof: $\widehat{P}^o_-$ is clearly not maximal symmetric and will therefore possess maximal symmetric extensions. Let $\widehat{B}$ be a maximal symmetric extension of $\widehat{P}^o_-$. Now

$$\begin{aligned} \widehat{B} \supset \widehat{P}^o_- &\implies \widehat{B}^\dagger \subseteq (\widehat{P}^o_-)^\dagger \\ &\implies (\widehat{B}^\dagger)^\dagger \supseteq ((\widehat{P}^o_-)^\dagger)^\dagger \\ &\implies \widehat{B} \supseteq \overline{\widehat{P}^o_-} \end{aligned} \tag{1.19}$$

since a maximal symmetric operator is necessarily closed. Introduce the operator $\widehat{P}_-$ defined on

$$\mathcal{D}(\widehat{P}_-) = \{\phi_- \in \mathcal{H}_- : \phi_- \in AC(\mathbb{R}^-_o), d\phi_-/dx \in \mathcal{H}_-, \phi_-(0^-) = 0\}$$

by

$$\widehat{P}_-\phi_- = -i\hbar\frac{d\phi_-}{dx},$$

where $\widehat{P}_-$ is maximal symmetric with adjoint $\widehat{P}^\dagger_-$ defined on

$$\mathcal{D}(\widehat{P}^\dagger_-) = \{\phi_- \in \mathcal{H}_- : \phi_- \in AC(\mathbb{R}^-_o), d\phi_-/dx \in \mathcal{H}_-\}$$

by

$$\widehat{P}^\dagger_-\phi_- = -i\hbar\frac{d\phi_-}{dx}$$

(cf. $\widehat{P}_+$ in appendix A). We now have

$$(\widehat{P}^o_-)^\dagger = \widehat{P}^\dagger_-$$

and so

$$((\widehat{P}^o_-)^\dagger)^\dagger = (\widehat{P}^\dagger_-)^\dagger,$$

i.e.

$$\overline{\widehat{P}^o_-} = \widehat{P}_-$$

as $\widehat{P}_-$ is maximal symmetric. Hence, by (1.19),

$$\widehat{B} \supseteq \widehat{P}_-,$$

i.e.

$$\widehat{B} = \widehat{P}_-.$$

We thus have a unique momentum operator in $L^2(\mathbb{R}_o^-)$, namely $\widehat{P}_-$. See appendix A for a generalisation of this result which invokes the notion of an essentially maximal symmetric operator.

In view of the analysis in section 1.5.1 we take the supercurrent operator for the left hand side to be

$$\widehat{J}_- = \frac{e}{\pi m}\widehat{P}_-.$$

Likewise we take

$$\widehat{J}_+ = \frac{e}{\pi m}\widehat{P}_+$$

to be the appropriate supercurrent operator for the right hand side.

Introduce the operator $\widehat{J}^o$ which is defined on $\mathcal{D}(\widehat{J}_-) \oplus \mathcal{D}(\widehat{J}_+)$ by

$$\widehat{J}^o = \widehat{J}_- \oplus \widehat{J}_+.$$

Now $\widehat{J}^o$ is a closed non-maximal symmetric operator which possesses a one parameter family of self-adjoint extensions $\{\widehat{J}_\lambda : \lambda \in (-\pi, \pi]\}$ where, for a given $\lambda \in (-\pi, \pi]$, $\widehat{J}_\lambda$ is defined by (appendix E)

$$\mathcal{D}(\widehat{J}_\lambda) = \left\{\phi \in L^2(\mathbb{R}_o^-) \oplus L^2(\mathbb{R}_o^+) : \phi_\pm \in AC(\mathbb{R}_o^\pm), d\phi_\pm/dx \in L^2(\mathbb{R}_o^\pm), \phi_-(0^-) = e^{-i\lambda}\phi_+(0^+)\right\}$$

and

$$\widehat{J}_\lambda \phi = -i\hbar\frac{e}{\pi m}\left(\frac{d\phi_-}{dx} \oplus \frac{d\phi_+}{dx}\right) \quad \forall \phi \in \mathcal{D}(\widehat{J}_\lambda),$$

where $\phi = \phi_- \oplus \phi_+$. Naturally, we assume that each $\widehat{J}_\lambda$ is a candidate supercurrent operator for the entire system.

Hamiltonian Operators

We start with the operator $\widehat{H}_+^o$ defined in $\mathcal{H}_+ \equiv L^2(\mathbb{R}_o^+)$ by

$$\mathcal{D}(\widehat{H}_+^o) = C_o^\infty(\mathbb{R}_o^+),$$

and

$$\widehat{H}_+^o \phi = -\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} \quad \forall \phi \in \mathcal{D}(\widehat{H}_+^o).$$

Now $\widehat{H}_+^o$ is symmetric with deficiency indices $(1,1)$ [50, p 144] and therefore admits a one parameter family of self-adjoint extensions. There is thus no unique Hamiltonian associated with the right hand side. We can define $\widehat{H}_-^o$ for the left hand side in a similar fashion, where $\widehat{H}_-^o$ also has deficiency indices $(1,1)$.

To obtain a Hamiltonian for the entire system we can either (i) choose a particular self-adjoint extension of $\widehat{H}_-^o$ and of $\widehat{H}_+^o$ then form their direct sum or (ii) form the direct sum of $\widehat{H}_-^o$ and $\widehat{H}_+^o$ and take the Hamiltonian to be a particular self-adjoint extension of the result. To keep our options open, we shall follow Exner and others [51, 52] by adopting the second scheme as this includes all extensions obtained via (i) anyway.[5] So we construct

$$\widehat{H}^o = \widehat{H}_-^o \oplus \widehat{H}_+^o$$

which is defined on

$$\mathcal{D}(\widehat{H}^o) = \mathcal{D}(\widehat{H}_-^o) \oplus \mathcal{D}(\widehat{H}_+^o).$$

The deficiency indices of $\widehat{H}^o$ are $(2,2)$ [42, p 149], and so $\widehat{H}^o$ possesses a four parameter family of self-adjoint extensions [32, p 155]. We shall assume that the superconductors on either side of the JJ are identical and that the effect of the JJ on a current is the same irrespective of the direction it is flowing. The relevant Hamiltonians then form a two-parameter family and two one-parameter families (appendix F). The two-parameter family is characterised by the boundary conditions

$$\phi_-(0^-) = -a\phi_-'(0^-) + b\phi_+'(0^+) \tag{1.20}$$

$$\phi_+(0^+) = a\phi_+'(0^+) - b\phi_-'(0^-) \tag{1.21}$$

where a and b are arbitrary real numbers and dashes represent differentiation. The two one-parameter families are characterised by the boundary conditions

$$\phi_-'(0^-) + \phi_+'(0^+) = 0 \tag{1.22}$$

$$\phi_-(0^-) + \phi_+(0^+) = c\Big(\phi_+'(0^+) - \phi_-'(0^-)\Big) \tag{1.23}$$

[5] We will have more to say about the scheme of Exner et al in section 1.5.3.

and

$$\phi'_-(0^-) = \phi'_+(0^+) \equiv \phi' \tag{1.24}$$

$$\phi_-(0^-) - \phi_+(0^+) = d\phi' \tag{1.25}$$

with $c \in \boldsymbol{R}$ and $d \in \boldsymbol{R} \cup \{\infty\}$.

We shall consider first the two-parameter family. Assuming $a^2 \neq b^2$ then eqns (1.20) and (1.21) may be transformed into

$$-\phi'_-(0^-) = A\phi_-(0^-) + B\phi_+(0^+) \tag{1.26}$$

$$\phi'_+(0^+) = A\phi_+(0^+) + B\phi_-(0^-) \tag{1.27}$$

where

$$A = \frac{a}{a^2 - b^2}, \qquad B = \frac{-b}{a^2 - b^2}. \tag{1.28}$$

We then identify the parameter B as the coupling coefficient and this is assumed to be uniquely determined by the JJ. Note that parameter b in (1.20) and (1.21) is not a suitable choice for the coupling coefficient as it is associated with the derivative of the wavefunction whereas coupling coefficients are generally taken to be associated with the wavefunction itself; cf. Feynman's original equations (appendix D). The case $a^2 = b^2$ will be considered later.

Now for a given $\lambda \in (-\pi, \pi]$, the set

$$\left\{\phi^\lambda_k = \phi^\lambda_{-k} \oplus \phi^\lambda_{+k} : k \in \boldsymbol{R}\right\},$$

where

$$\phi^\lambda_{-k}(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

and

$$\phi^\lambda_{+k}(x) = \frac{1}{\sqrt{2\pi}} e^{i(kx+\lambda)}$$

is an orthogonal complete set of generalised eigenfunctions of $\widehat{J}_\lambda$. To each ϕ^λ_k, the corresponding current eigenvalue is $e\hbar k/\pi m$.

If ϕ_k^λ is to be the state of a steady supercurrent then it must also be an eigenstate of the (as yet undetermined) Hamiltonian. Let $\widetilde{H}$ be an arbitrary self-adjoint extension of $\widehat{H}^o$ so that

$$\widehat{H}^o \subset \widetilde{H} \Longrightarrow \widetilde{H}^\dagger \subseteq (\widehat{H}^o)^\dagger. \tag{1.29}$$

As $(\widehat{H}^o)^\dagger = (\widehat{H}^o_-)^\dagger \oplus (\widehat{H}^o_+)^\dagger$ and $(\widehat{H}^o_\pm)^\dagger$ acts as $-(-\hbar^2/2m)d^2/dx^2$ ([42, p 145],[53]), then (1.29) tells us that $\widetilde{H}$ has the same formal expression as $\widehat{H}^o$, and since

$$-\frac{\hbar^2}{2m}\frac{d^2\phi^\lambda_{\pm k}}{dx^2} = \frac{\hbar^2 k^2}{2m}\phi^\lambda_{\pm k},$$

then ϕ_k^λ is a formal eigenfunction of all possible Hamiltonians. To ensure ϕ_k^λ is a generalised eigenfunction in the usual sense it must also be (locally) in the domain of the Hamiltonian. For those Hamiltonians parametrised by A and B, ϕ_k^λ is required to satisfy boundary conditions (1.26) and (1.27). So, into eqns (1.26) and (1.27), we substitute

$$\phi_-(x) = \phi^\lambda_{-k}(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}$$

and

$$\phi_+(x) = \phi^\lambda_{+k}(x) = \frac{1}{\sqrt{2\pi}}e^{i(kx+\lambda)}$$

to obtain

$$-ik = A + Be^{i\lambda} \tag{1.30}$$

$$ike^{i\lambda} = Ae^{i\lambda} + B. \tag{1.31}$$

Equating real and imaginary parts of eqn (1.30) yields

$$0 = A + B\cos\lambda \tag{1.32}$$

$$-k = B\sin\lambda. \tag{1.33}$$

Likewise for eqn (1.31) we have

$$-k\sin\lambda = A\cos\lambda + B \tag{1.34}$$

$$k\cos\lambda = A\sin\lambda. \tag{1.35}$$

From eqn (1.32) we have $A = -B\cos\lambda$. Substituting this into eqns (1.34) and (1.35) yields (1.33) in each case. So eqns (1.34) and (1.35) give us no more information about A and B than do eqns (1.32) and (1.33), and thus serve only as a consistency check.

Now as B is assumed to be a fixed characteristic of the JJ then it should have no k dependence, and since to each $\lambda \in (-\pi, \pi]$ there corresponds a different supercurrent operator for the same JJ then B would also have to be independent of λ. We then see that eqn (1.33) is essentially Josephson's equation. To be precise, we have

$$j_k = j_o \sin\lambda \tag{1.36}$$

where $j_k = e\hbar k/\pi m$ and $j_o = -e\hbar B/\pi m$.

For a particular JJ, a given value of λ determines a unique Hamiltonian, since $A = -B\cos\lambda$. Clearly, $A^2 = B^2$ if $\lambda \in \{0, \pi\}$ but it is obvious from (1.28) that $a^2 \neq b^2 \Rightarrow A^2 \neq B^2$ and it follows that eqn (1.36) is not valid for $\lambda \in \{0, \pi\}$. This problem is easily remedied. We can verify that ϕ_k^λ, for arbitrary $\lambda \in (-\pi, \pi]$ and arbitrary $k \in \mathbb{R}$, does not solve eqns (1.20) and (1.21) if $a^2 = b^2$. Firstly, if $a = b$, then we have $\phi_+(0^+) = \phi_-(0^-)$ and so $exp(i\lambda) = 1$, i.e. $\lambda = 0$, whereas by equating the real parts of the left and right hand sides of eqn (1.20) upon the substitution of ϕ_k^λ, we have $1 = -ak\sin\lambda$. This contradiction means that those Hamiltonians for which $a = b$ do not admit generalised eigenfunctions which are permissible superconducting states. Likewise, we reach the same conclusion for $a = -b$. We may therefore extend the validity of eqn (1.36) to include $\lambda = 0$ and $\lambda = \pi$ since j_k is then zero for such values and no supercurrent flows across the JJ.

To support our claim that B should be held constant while A be permitted to vary with λ, we shall suppose instead that A is fixed. By eqn (1.32), B must be equated with $-A/\cos\lambda$ and we arrive at the Josephson type equation $k = A\tan\lambda$. However, this alternative approach is problematic. Clearly k is not bounded, which would allow arbitrarily large currents; such behaviour is unacceptable as all superconductors have a finite critical current beyond which superconductivity is destroyed.

We have still to deal with the two one-parameter families specified by (1.22,1.23) and (1.24,1.25). Substituting ϕ_k^λ into (1.22) yields $exp(i\lambda) = -1$, i.e. $\lambda = \pi$. Substituting

ϕ_k^λ, with $\lambda = \pi$, into (1.23) yields $c = 0$. Similarly, if we substitute ϕ_k^λ into (1.24) and (1.25), we obtain $\lambda = 0$ and $d = 0$. Thus, in addition to our two-parameter family of Hamiltonians, we have two extra Hamiltonians, each of which possesses eigenfunctions shared by a corresponding supercurrent operator. Note that for either of these additional Hamiltonians, there is no restriction on k. In particular, k need not be zero even though $\sin\lambda$ is zero for $\lambda = 0$ and $\lambda = \pi$. This behaviour is not characteristic of the presence of a JJ and we therefore conclude that the two one-parameter families of Hamiltonians are not applicable to the system under study. Also, the boundary conditions (1.22,1.23) and (1.24,1.25) can be obtained as limiting cases of the boundary conditions (1.20,1.21) and in this sense can be regarded as characterising exceptional Hamiltonians [53]. To substantiate this we note that the Hamiltonian identified by (1.24,1.25) with $d = 0$ corresponds to the free particle Hamiltonian, and in this case the JJ would be considered absent.

1.5.3 Quantisation by Parts

The means by which we obtained the family of supercurrent operators $\{\widehat{J}_\lambda : \lambda \in (-\pi, \pi]\}$ for the system of an infinitely long superconductor containing a single JJ can be considered as an application of the method of 'quantisation by parts' recently proposed by Harrison and Wan [47]. This scheme applies to systems which have a circuit configuration. It is assumed that each component part of the circuit has enough integrity to deserve to be a quasi-system of its own. Each of these parts is therefore quantised separately; the whole system is then quantised by adding up these separately quantised parts together in some sense. In what sense? This depends on the particular system. For the superconductor containing a JJ we simply took the direct sum of the left and right hand current operators and found its maximal symmetric extensions. The situation is different for the current-fed TSCR. For now we ignore the leads as in [47]. The total-current operator for the TSCR will not be $\widehat{J}_{\varphi_l} \oplus \widehat{J}_{\varphi_u} \equiv \widehat{J}_\varphi$, where $\varphi_l = \varphi_u = \varphi$. This is because an input current I determines the state of the system, namely $\psi_I^l \oplus \psi_I^u \equiv \psi_I$, and clearly $\widehat{J}_\varphi \psi_I = (I/2)\psi_I$, whereas we would want the eigenvalue of the total-current operator corresponding to eigenfunction

ψ_I to be I. We overcome this problem by first extending the operators $\widehat{J}_{\varphi_l}$ and $\widehat{J}_{\varphi_u}$ to operators in the Hilbert space for the entire ring, i.e. $\mathcal{H}_l \oplus \mathcal{H}_u \equiv \mathcal{H}_R$. Define $\widehat{J}^l_\varphi$ and $\widehat{J}^u_\varphi$ by

$$\widehat{J}^l_\varphi = \widehat{J}_{\varphi_l} \oplus \frac{I}{2}\widehat{\mathcal{I}}_u; \quad \widehat{J}^u_\varphi = \frac{I}{2}\widehat{\mathcal{I}}_l \oplus \widehat{J}_{\varphi_u}; \qquad (\varphi = \varphi_l = \varphi_u),$$

where $\widehat{\mathcal{I}}_u$ and $\widehat{\mathcal{I}}_l$ are the identity operators on $\mathcal{H}_u$ and $\mathcal{H}_l$ respectively, so that

$$\widehat{J}^l_\varphi \psi_I = \widehat{J}^u_\varphi \psi_I = \frac{I}{2}\psi_I.$$

Now the operator $\widehat{J}^t_\varphi$ defined by

$$\widehat{J}^t_\varphi \equiv \widehat{J}^l_\varphi + \widehat{J}^u_\varphi$$

satisfies

$$\widehat{J}^t_\varphi \psi_I = I\psi_I$$

and it is $\widehat{J}^t_\varphi$ which is taken in [47] to be the appropriate total current operator for the ring.

Clearly, the sense in which we 'add up' separately quantised circuit components in series, such as in the example of an infinite superconducting wire containing a JJ, is different to the way we 'add up' the separately quantised components in a parallel circuit like the upper and lower sections of the TSCR. So, as a general rule, we expect that for series circuits, direct sums are appropriate since the eigenvalues can be preserved and for parallel circuits, standard summations are appropriate since eigenvalues are added together.

As promised in section 1.5.1, we shall now determine a supercurrent operator for the entire ring + leads system using the method of quantisation by parts outlined above. As the ring and leads are in series, we take our provisional 'global' supercurrent-operator to be $\widehat{J}^o_\varphi$ where

$$\widehat{J}^o_\varphi = \widehat{J}_{in} \oplus \widehat{J}_{out} \oplus \widehat{J}^t_\varphi.$$

Since $\widehat{J}^t_\varphi$ is self-adjoint with deficiency indices $(0,0)$ and each of $\widehat{J}_{in}$ and $\widehat{J}_{out}$ is maximal symmetric with respective deficiency indices $(0,1)$ and $(1,0)$ (cf. appendix E), then $\widehat{J}^o_\varphi$ is a closed symmetric operator with deficiency indices $(1,1)$ [42, pp 145,149]. Therefore

$\widehat{J}^o_\varphi$ possesses a one parameter family of self-adjoint extensions. Firstly, we shall determine the self-adjoint extensions of the operator $\widehat{J}^{l_o} \equiv \widehat{J}_{in} \oplus \widehat{J}_{out}$, which is associated with the leads only and is likewise closed, symmetric and has deficiency indices $(1, 1)$. The direct sums of each of these extensions with $\widehat{J}^t_\varphi$ then comprises the family of self-adjoint extensions of $\widehat{J}^o_\varphi$. Now the self-adjoint extensions of $\widehat{J}^{l_o}$ constitute the one parameter family $\left\{\widehat{J}^l_\lambda : \lambda \in (-\pi, \pi]\right\}$ where, for a given λ, we have

$$\begin{aligned} \mathcal{D}(\widehat{J}^l_\lambda) = \{\phi = \phi_- \oplus \phi_+ \in L^2(\mathbb{R}_{-a}) \oplus L^2(\mathbb{R}_{+a}) : \phi_\pm &\in AC(\mathbb{R}_{\pm a}), \\ \phi'_\pm &\in L^2(\mathbb{R}_{\pm a}), \phi_-(-a) = e^{-i\lambda}\phi_+(a)\} \end{aligned}$$

and

$$\widehat{J}^l_\lambda \phi = -i\hbar \frac{e}{\pi m}(\phi'_- \oplus \phi'_+) \quad \forall \phi \in \mathcal{D}(\widehat{J}^l_\lambda).$$

The proof of this is essentially that in appendix E. Hence, the family $\{\widehat{J}_{\varphi\lambda} : \lambda \in (-\pi, \pi]\}$ where

$$\widehat{J}_{\varphi\lambda} = \widehat{J}^l_\lambda \oplus \widehat{J}^t_\varphi,$$

is the desired family of self-adjoint extensions of $\widehat{J}^o_\varphi$. It is clear that the single valuedness condition can now be extended to the entire system provided $\lambda = \varphi$ and so the current magnitude I, which determines a unique value for φ, also determines a unique global current-operator $\widehat{J}_I \equiv \widehat{J}_{\varphi\lambda}$ (where $\lambda = \varphi \Leftarrow I$).

Quantisation by Parts versus the Scheme of Exner et al

We wish to compare and contrast the method of quantisation by parts with a similar scheme that also finds application to systems which have a circuit configuration. The scheme in question is due to Exner and co-workers [42, 51, 52, 53] and will from now on be referred to as Exner's method. To date, Exner's method appears to have been used only to find Hamiltonians, though there is no reason why it could not be extended to other observables such as momentum. Staying with Hamiltonians for the time being, the crux of Exner's method can be understood by reviewing the construction of the 'Josephson effect Hamiltonians' in section 1.5.2. From the outset, it was assumed that the Josephson junction could be ignored and that its presence would be reflected in an appropriate choice of Hamiltonian for the remaining two-component system. The candidate Hamiltonians for the two-component system, i.e. the two superconductors, were obtained in three distinct stages. In the first stage we identified the left and right hand superconductors with the Hilbert spaces $L^2(\mathbb{R}_o^-)$ and $L^2(\mathbb{R}_o^+)$ respectively. The operators $\widehat{H}_-^o$ and $\widehat{H}_+^o$ were then introduced, where $\widehat{H}_\pm^o$ is defined in $L^2(\mathbb{R}_o^\pm)$ by $\widehat{H}_\pm^o = -(\hbar^2/2m)d^2/dx^2$ on domain $C_o^\infty(\mathbb{R}_o^\pm)$ and is symmetric with deficiency indices $(1,1)$. The second stage involved taking the direct sum of $L^2(\mathbb{R}_o^-)$ and $L^2(\mathbb{R}_o^+)$ and identifying the resulting Hilbert space with the entire system. We also formed the direct sum of $\widehat{H}_-^o$ and $\widehat{H}_+^o$. This yielded the symmetric operator $\widehat{H}^o$ which has deficiency indices $(2,2)$. The final stage required us to extend $\widehat{H}^o$ to a self-adjoint operator. In this case there were uncountably many self-adjoint extensions, each one being a candidate for the Hamiltonian for the entire system.

Exner's method can be applied to more complex configurations than the two-component circuit being considered here. Typically, the spatial manifold on which a particle moves is broken up into simpler submanifolds and the Hamiltonians for the entire system are obtained by following a procedure analogous to that for the example above. The crucial difference between the method of quantisation by parts and Exner's method is that quantisation by parts involves quantising each component of the system separately and then summing up these separately quantised parts, whereas Exner's method associates an observable only with the entire circuit and this is obtained at the very end of the quantisation procedure. Clearly, quantisation by parts is more suited to those systems for which it is meaningful to consider observable values associated with its various component parts. The current-fed TSCR is an example of just such a system. The current flowing through the circuit behaves classically and the bisected input current results in a definite value for the current flowing through each half of the ring.

If we extend Exner's method so that it caters for momentum operators and thus current-operators, we can apply it to the current-fed TSCR (minus leads). One of the resulting candidates for the total-current operator would be the self-adjoint operator $\widehat{J}_\varphi \equiv$

$\widehat{J}_{\varphi_l} \oplus \widehat{J}_{\varphi_u}$ given earlier. However, as we have seen, the eigenfunctions of this operator cannot be identified with a total current I and simultaneously with a current $I/2$ in each of the two halves of the ring. For series circuits though, like the system of two superconductors separated by a Josephson junction, Exner's method includes the method of quantisation by parts as a special case. Indeed, for this particular system, the Hamiltonian operators cannot be obtained by the quantisation by parts method and this is why 'keeping our options open' in section 1.5.2 paid off.

The reason why, especially within the context of orthodox quantum mechanics, Exner's method generally gives more candidate observables for a circuit system than the method of quantisation by parts is that in a direct sum of symmetric operators the deficiency indices add. A self-adjoint extension of such a sum will in general have states in its domain which correlate different component parts of the circuit. On the other hand, a direct sum of self-adjoint operators is self-adjoint and cannot be extended further, so no such 'mixed boundary conditions' need to be imposed. However, within the context of our generalised theory, 'the whole can be greater than the sum of its parts' for the method of quantisation by parts as well. This is because a direct sum of maximal symmetric operators need not be maximal symmetric and it becomes necessary to add an extra stage to the method of quantisation by parts in which we determine maximal symmetric extensions. We have already assumed this extra stage when we determined the current-operators in the derivation of Josephson's equation for the system of two superconductors separated by a Josephson junction. Incidently, for this particular system, the method of quantisation by parts and Exner's method yield the same set of current-operators. Also, it is interesting to note that for this example Exner's method applies within the context of orthodox quantum mechanics, since only the resulting self-adjoint extensions $\{\widehat{J}_\lambda : \lambda \in (-\pi, \pi]\}$ are regarded as observables; the intermediate operators $\widehat{J}_-$ and $\widehat{J}_+$ are not attributed physical meaning.

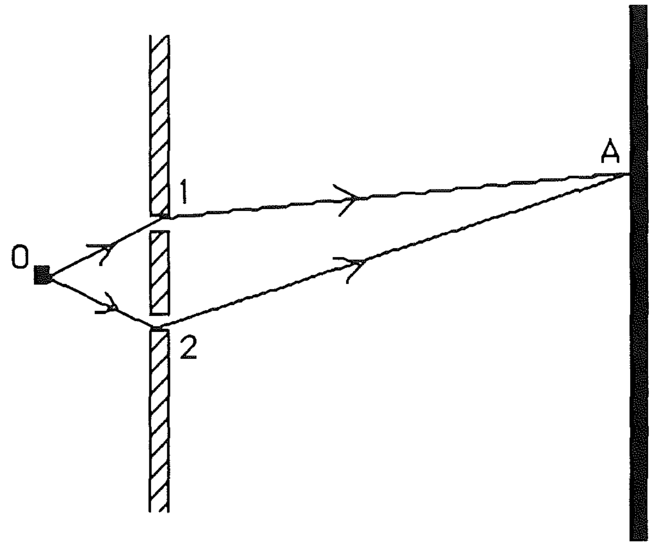

Figure 1.2: Double Slit Interference Experiment

1.5.4 Double Slit Interference with Electrons

We shall attempt to apply the method of quantisation by parts, introduced in [47] to describe the macroscopic quantum system of a current-fed thick superconducting ring (TSCR), to a microscopic system. Specifically, we wish to formulate a description of a quantum particle, say an electron, which passes through the double slit configuration shown in figure 1.2. The resulting model, when compared with that of the current-fed TSCR, can be used to highlight some of the differences between macroscopic and microscopic quantum systems.

We start with a classical system consisting of a single particle which leaves the point O and arrives at a point A on the screen by taking either one or the other of the two paths shown. Path 1 is identified with the interval $\Omega_1 = [0, \omega_1]$ and path 2 with the interval $\Omega_2 = [\omega_1, \omega_2]$. The paths can be coordinated by the position variables x_1 and x_2 so that the points $x_1 = 0$ and $x_2 = \omega_2$ coincide with O and also $x_1 = \omega_1$ and $x_2 = \omega_1$ coincide with A.

The classical motion on each path is to be quantised separately. For path 1 the appropriate Hilbert space is taken to be $\mathcal{H}_1 = L^2(\Omega_1, dx_1)$ and the canonical momentum is quantised as the self-adjoint operator $\widehat{p}_{\varphi_1}$ which is defined by

$$\mathcal{D}(\widehat{p}_{\varphi_1}) = \left\{\phi_1 \in \mathcal{H}_1 : \phi_1 \in AC(\Omega_1), \phi_1^{'} \in \mathcal{H}_1, \phi_1(0) = e^{-i\varphi_1}\phi_1(\omega_1)\right\}$$

$$\widehat{p}_{\varphi_1}\phi_1 = -i\hbar\frac{d\phi_1}{dx_1} \quad \forall\phi_1 \in \mathcal{D}(\widehat{p}_{\varphi_1}),$$

where φ_1 is an arbitrary real number.

The eigenfunctions of $\widehat{p}_{\varphi_1}$ are given by

$$\phi^1_{\varphi_1 n_1}(x_1) = \frac{1}{\sqrt{\omega_1}}e^{\imath P_{\varphi_1 n_1}x_1} \qquad \imath = i/\hbar$$

with corresponding eigenvalues

$$P_{\varphi_1 n_1} = (2\pi n_1 + \varphi_1)\frac{\hbar}{\omega_1}.$$

Likewise, for path 2 we can introduce the analogously defined Hilbert space $\mathcal{H}_2$ and momentum operator $\widehat{p}_{\varphi_2}$ with eigenfunctions $\phi^2_{\varphi_2 n_2}$ and eigenvalues $P_{\varphi_2 n_2}$. These are:

$$\mathcal{H}_2 = L^2(\Omega_2, dx_2),$$

$$\mathcal{D}(\widehat{p}_{\varphi_2}) = \left\{\phi_2 \in \mathcal{H}_2 : \phi_2 \in AC(\Omega_2), \phi_2^{'} \in \mathcal{H}_2, \phi_2(\omega_1) = e^{i\varphi_2}\phi_2(\omega_2)\right\}$$

$$\widehat{p}_{\varphi_2}\phi_2 = -i\hbar\frac{d\phi_2}{dx_2} \quad \forall\phi_2 \in \mathcal{D}(\widehat{p}_{\varphi_2}),$$

where φ_2 is an arbitrary real number;

$$\phi^2_{\varphi_2 n_2}(x_2) = \frac{1}{\sqrt{\omega_2 - \omega_1}}e^{\imath P_{\varphi_2 n_2}(\omega_2 - x_2)},$$

$$P_{\varphi_2 n_2} = (2\pi n_2 + \varphi_2)\frac{\hbar}{\omega_2 - \omega_1}.$$

Notice that in defining $\phi^2_{\varphi_2 n_2}(x_2)$, the arbitrary multiplicative phase factor has been set so that the condition

$$\phi^1_{\varphi_1 n_1}(0) = \phi^2_{\varphi_2 n_2}(\omega_2) \tag{1.37}$$

is satisfied for $\omega_2 = 2\omega_1$, i.e. for the case where the path lengths are equal. However, we generally do not have

$$\phi^1_{\varphi_1 n_1}(\omega_1) = \phi^2_{\varphi_2 n_2}(\omega_1), \tag{1.38}$$

as this would require $P_{\varphi_1 n_1}$ and $P_{\varphi_2 n_2}$ to coincide. For the current-fed TSCR depicted in figure 1.1, the eigenvalues of the current-operators associated with the upper and lower halves of the ring are uniquely determined by the input current due to its classical behaviour and this is why single valuedness conditions analogous to both (1.37) and (1.38) could be established for that system.

A general electron state for the double slit configuration would not correspond to the electron following one path only. The problem now is to cater for such states. Introduce the Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 = L^2(\Omega, dx)$, where Ω is the interval $[0, \omega_2] = \Omega_1 \cup \Omega_2$ coordinated by a position variable x. A general electron state is assumed to be an element of $\mathcal{H}$.

Observables pertaining to only one path are to be represented by an appropriate extension to $\mathcal{H}$. Denote the set $\Omega_1 - \{0, \omega_1\}$ by Ω_1^o, i.e. Ω_1^o is the interval $(0, \omega_1)$ and similarly $\Omega_2^o \equiv \Omega_2 - \{\omega_1, \omega_2\} = (\omega_1, \omega_2)$. We can now decompose $\mathcal{H}$ thus:

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2^o = \mathcal{H}_1^o \oplus \mathcal{H}_2,$$

where $\mathcal{H}_1^o = L^2(\Omega_1^o)$ and $\mathcal{H}_2^o = L^2(\Omega_2^o)$. Let $\widehat{O}_2^o$ be the zero operator on $\mathcal{H}_2^o$. The operator $\widehat{P}_{\varphi_1}$ defined on

$$\mathcal{D}(\widehat{P}_{\varphi_1}) = \mathcal{D}(\widehat{p}_{\varphi_1}) \oplus \mathcal{H}_2^o$$

by

$$\widehat{P}_{\varphi_1} = \widehat{p}_{\varphi_1} \oplus \widehat{O}_2^o$$

is self-adjoint in $\mathcal{H}$ [42, p 145] and we take $\widehat{P}_{\varphi_1}$ to be the appropriate extension of $\widehat{p}_{\varphi_1}$ to $\mathcal{H}$. Note that $\widehat{P}_{\varphi_1}$ has the same spectrum as $\widehat{p}_{\varphi_1}$ with an additional infinitely degenerate eigenvalue of zero, i.e.

$$\widehat{P}_{\varphi_1}(\phi^1_{\varphi_1 n_1} \oplus \emptyset_2^o) = P_{\varphi_1 n_1}(\phi^1_{\varphi_1 n_1} \oplus \emptyset_2^o)$$

and

$$\widehat{P}_{\varphi_1}(\emptyset_1^o \oplus \psi_2) = 0(\emptyset_1^o \oplus \psi_2)$$

where $\emptyset_1^o$ and $\emptyset_2^o$ are the zero vectors in $\mathcal{H}_1^o$ and $\mathcal{H}_2^o$ respectively and ψ_2 is an arbitrary element of $\mathcal{H}_2$. Likewise we can define $\widehat{P}_{\varphi_2} = \widehat{O}_1^o \oplus \widehat{p}_{\varphi_2}$ etc. The zero eigenvalues arise because, by extending the description to take into account both paths, we allow the possibility that the electron can follow one path or the other. An eigenfunction of $\widehat{P}_{\varphi_1}$ associated with an eigenvalue of zero represents an electron confined to path 2. Similarly, an eigenfunction of $\widehat{P}_{\varphi_2}$ associated with an eigenvalue of zero represents an electron confined to path 1. Contrast this with the behaviour of the classical current in Harrison and Wan's model of a current-fed TSCR where the current always splits up so that it has a non-zero component in each path.

In order to achieve an interference pattern on the screen we superpose eigenstates of $\widehat{P}_{\varphi_1}$ and $\widehat{P}_{\varphi_2}$ associated with the same non-zero momentum magnitude $k > 0$, i.e. $k = P_{\varphi_1 n_1} = -P_{\varphi_2 n_2}$. Here, $P_{\varphi_2 n_2}$ is negative because an electron following path 2 to the screen travels in the direction of decreasing x_2. We may now replace the subscripts $\varphi_1 n_1$ and $\varphi_2 n_2$ with a k.

Let $\phi_k^{(1)}$ and $\phi_k^{(2)}$ be elements of $\mathcal{H}$ defined by

$$\phi_k^{(1)} = \phi_k^1 \oplus \emptyset_2^o$$

and

$$\phi_k^{(2)} = \emptyset_1^o \oplus \phi_k^2,$$

i.e.

$$\phi_k^{(1)}(x) = \begin{cases} \phi_k^1(x) & x \in [0, \omega_1] \\ 0 & x \in (\omega_1, \omega_2) \end{cases}$$

and

$$\phi_k^{(2)}(x) = \begin{cases} 0 & x \in (0, \omega_1) \\ \phi_k^2(x) & x \in [\omega_1, \omega_2]. \end{cases}$$

Now superpose $\phi_k^{(1)}$ and $\phi_k^{(2)}$ thus

$$\phi_k \equiv \alpha_1 \phi_k^{(1)} + \alpha_2 \phi_k^{(2)}.$$

If $|\alpha_1| = 1$ and $\alpha_2 = 0$ then ϕ_k describes an electron which follows path 1 to the screen with momentum k. Likewise if $\alpha_1 = 0$ and $|\alpha_2| = 1$ then ϕ_k describes an electron which follows path 2 to the screen with momentum k. We shall assume $\alpha_1 = \alpha_2 = 1/\sqrt{2}$, so that

$$|\phi_k(x)|^2 = \begin{cases} \frac{1}{2}|\phi_k^1(x)|^2 = \frac{1}{2\omega_1} & x \in [0, \omega_1) \\ \frac{1}{2}|\phi_k^2(x)|^2 = \frac{1}{2(\omega_2 - \omega_1)} & x \in (\omega_1, \omega_2] \end{cases}$$

and

$$
\begin{aligned}
|\phi_k(\omega_1)|^2 &= \frac{1}{2}|\phi_k^1(\omega_1)|^2 + \frac{1}{2}|\phi_k^2(\omega_1)|^2 + Re\left[\left(\phi_k^1(\omega_1)\right)^* \phi_k^2(\omega_1)\right] \\
&= \frac{1}{2\omega_1} + \frac{1}{2(\omega_2-\omega_1)} + \frac{1}{2\sqrt{\omega_1(\omega_2-\omega_1)}}\left(e^{\frac{i}{\hbar}k(\omega_2-2\omega_1)} + e^{-\frac{i}{\hbar}k(\omega_2-2\omega_1)}\right) \\
&= \frac{1}{2\omega_1} + \frac{1}{2(\omega_2-\omega_1)} + \frac{1}{\sqrt{\omega_1(\omega_2-\omega_1)}}\cos\left(\frac{k}{\hbar}|\omega_2-2\omega_1|\right),
\end{aligned}
$$

where $|\omega_2 - 2\omega_1|$ is just the difference in the path lengths.

This description is valid only for fixed A, i.e. fixed ω_1 and ω_2. If we want to build up the interference pattern on the screen we must change the system, i.e. we quantise the classical system of a particle which can follow one of two new paths, both of which lead to a point A' say, on the screen. Notice that we only have interference at the screen and nowhere else, this is to be contrasted with the standard treatment where there is interference everywhere. Also, unlike in Feynman's sum over paths (SOP) approach, interference at A is obtained by considering two electron paths only. In our model, the paths are determined by the dynamics of a classical particle which travels from O to A. In the SOP picture, interference at A is interpreted as a weighted sum over all the alternative paths from O to A [54, pp 69–74].

For the current-fed TSCR there is no analogous interference effect. If the recombination point, i.e. the point on the ring where the output lead is connected, is located at $\theta = \theta_o$, then θ_o is akin to the interference point A on the screen of the double slit experiment. In [47] it is shown that a single valuedness condition corresponding to (1.38) can be imposed regardless of what θ_o is. This is possible because the eigenvalues, and thus the eigenfunctions, of the current-operators associated with the upper and lower halves of the ring depend on both the input current I and the angle θ_o. It turns out that the nature of this dependence implies the single valuedness condition corresponding to (1.38).

To conclude then, we can obtain a description of an electron which passes through a double slit configuration by applying the method of quantisation by parts to the classical system of a particle which can take one of two paths, each of which is uniquely defined by one of the slits and the point of arrival on the screen. Superposing a state $\phi_k^{(1)}$, associated with an electron travelling to the screen with momentum k via path 1, and a state $\phi_k^{(2)}$, associated with an electron travelling to the screen with momentum k via path 2, yields the well known interference pattern on the screen. This is to be contrasted with the behaviour of a current-fed TSCR, where the absence of an analogous interference effect is due to the classical nature of the current.

Appendix A: Symmetric Operators and Generalised Spectral Functions

This appendix is largely a review of the relevant mathematics we require in order to proceed with our analysis. We shall highlight and compare specific properties of different symmetric operators, the particular reasons for doing so will become clear when the physical implications are considered.

The main references for this appendix are [11, app. I], [55, ch. XII] and [56, ch. 10].

Symmetric Operators and their Extensions

Definition 4 *A linear operator $\widehat{A}$ defined on domain $\mathcal{D}(\widehat{A})$ in a Hilbert space $\mathcal{H}$ is said to be symmetric if and only if $\mathcal{D}(\widehat{A})$ is dense in $\mathcal{H}$ and*

$$\widehat{A}^{\dagger} \supseteq \widehat{A}.$$

If the equality holds then $\widehat{A}$ is said to be self-adjoint.

Example: Let J be an interval $[a, b]$ of $\boldsymbol{R}$. The operator $\widehat{P}_o(J) = -i\hbar d/dx$ defined in $L^2(J)$ on the dense domain

$$\mathcal{D}(\widehat{P}_o(J)) = \{\phi \in L^2(J) : \phi \in AC(J),\, d\phi/dx \in L^2(J),\, \phi(a) = \phi(b) = 0\}$$

has adjoint $\widehat{P}_o^\dagger(J) = -i\hbar d/dx$ defined on

$$\mathcal{D}(\widehat{P}_o^\dagger(J)) = \{\phi \in L^2(J) : \phi \in AC(J),\, d\phi/dx \in L^2(J)\},$$

i.e. $\widehat{P}_o^\dagger(J) \supset \widehat{P}_o(J)$ and $\widehat{P}_o(J)$ is symmetric.[6]

Example: The operator $\widehat{P}^\lambda(J) = -i\hbar d/dx$ defined on the dense domain

$$\mathcal{D}(\widehat{P}^\lambda(J)) = \{\phi \in L^2(J) : \phi \in AC(J),\, d\phi/dx \in L^2(J),\, \phi(a) = e^{-i\lambda}\phi(b)\},$$

where λ is an arbitrary real number, coincides with its adjoint and so is self-adjoint.

A property of symmetric operators which plays an important role throughout this thesis is their extendibility.

Definition 5 *If $\widehat{A}$ is a symmetric operator defined in a Hilbert space $\mathcal{H}$ and $\widehat{B}^+$ is a symmetric operator defined in a Hilbert space $\mathcal{H}^+ \supseteq \mathcal{H}$ such that $\widehat{B}^+ \supseteq \widehat{A}$ then $\widehat{B}^+$ is called a generalised symmetric extension of $\widehat{A}$. If $\widehat{B}^+ \supset \widehat{A}$ then $\widehat{B}^+$ is called a proper generalised symmetric extension.*

There are two types of generalised extension which will be of particular interest to us; these can be classified thus:

$$(1) \qquad \mathcal{D}(\widehat{A}) \neq \mathcal{D}(\widehat{B}^+) \cap \mathcal{H} = \mathcal{D}(\widehat{B}^+),$$

$$(2) \qquad \mathcal{D}(\widehat{A}) = \mathcal{D}(\widehat{B}^+) \cap \mathcal{H} \neq \mathcal{D}(\widehat{B}^+).$$

Type (1) extensions are seen to be the familiar 'extensions in the same space'.

Example: The operator $\widehat{P}^\lambda(J)$ is a type (1) extension of $\widehat{P}_o(J)$.

[6]Let Λ be an interval (not necessarily finite) of $\mathbb{R}$. The set $AC(\Lambda)$ denotes the set of functions which are absolutely continuous in Λ. In other words $\phi \in AC(\Lambda)$ if and only if ϕ' exists a.e. and is integrable on every bounded interval in Λ, and, for $a, b \in \Lambda$ such that $a < b$,

$$\phi(b) - \phi(a) = \int_a^b \phi'(x)dx.$$

To obtain a type (2) extension it is necessary to 'leave the space'.

Example: The operator $\widehat{P}$ defined on

$$\mathcal{D}(\widehat{P}) = \{\phi \in L^2(\mathbb{R}) : \phi \in AC(\mathbb{R}),\ \phi' \in L^2(\mathbb{R})\}$$

by

$$\widehat{P}\phi = -i\hbar\frac{d\phi}{dx}$$

is a type (2) extension of $\widehat{P}_o(J)$, where $\mathcal{H}^+ = L^2(\mathbb{R})$ and $\mathcal{H} = L^2(J)$.

To see this, an arbitray $\phi \in \mathcal{H}$ is identified with $\phi^+ \in \mathcal{H}^+$ where $\phi^+(x) = \phi(x)$ for $x \in J$ and $\phi^+(x) = 0$ for $x \notin J$, so then $\phi \in \mathcal{D}(\widehat{P}) \cap \mathcal{H}$ if and only if $\phi \in AC(J)$ and $\phi(a) = \phi(b) = 0$.

Definition 6 *If a symmetric operator has type (2) symmetric extensions only, then it is called maximal symmetric.*

Example: The operator $\widehat{P}_+$ defined by

$$\mathcal{D}(\widehat{P}_+) = \left\{\phi \in L^2(\mathbb{R}^+) : \phi \in AC(\mathbb{R}^+), \phi' \in L^2(\mathbb{R}^+), \phi(0) = 0\right\}$$

and

$$\widehat{P}_+\phi = -i\hbar\frac{d\phi}{dx} \quad \forall\phi \in \mathcal{D}(\widehat{P}_+)$$

is maximal symmetric in $L^2(\mathbb{R}^+)$.

Theorem 3 *Every symmetric operator has a maximal symmetric type (1) extension.*

Theorem 4 *Every symmetric operator has a self-adjoint type (2) extension.*

Hereafter a type (1) extension will be referred to simply as an extension. Extensions not of type (1) will be called extensions with exit, these include type (2) extensions.

An invaluable tool for investigating the existence and nature of proper symmetric extensions (i.e. proper type (1) extensions) of a symmetric operator is the method of deficiency indices [55, p 1226], [56, p 254].

Definition 7 *Let $\widehat{A}$ be a symmetric operator and define the positive and negative deficiency spaces of $\widehat{A}$ by*

$$N_+ \equiv \left\{ \phi \in \mathcal{D}(\widehat{A}^\dagger) : \widehat{A}^\dagger \phi = i\phi \right\}$$

and

$$N_- \equiv \left\{ \phi \in \mathcal{D}(\widehat{A}^\dagger) : \widehat{A}^\dagger \phi = -i\phi \right\}$$

respectively. Their dimensions, denoted by n_+ and n_-, are called the positive and negative deficiency indices of $\widehat{A}$ and are usually written as the ordered pair (n_+, n_-).

Clearly, if $\widehat{A}$ is a symmetric operator with deficiency indices (n_+, n_-) then the operator $-\widehat{A}$, which has adjoint $-\widehat{A}^\dagger$, is symmetric with deficiency indices (n_-, n_+).

Theorem 5 *A closed symmetric operator $\widehat{A}$ possesses a proper symmetric extension if and only if both n_+ and n_- are non-zero. In other words $\widehat{A}$ is maximal symmetric if and only if at least one of its deficiency indices is zero.*

Example: The operator $\widehat{P}_o(J)$ has deficiency indices (1,1) and has a proper symmetric extension $\widehat{P}^\lambda(J)$ which in turn has deficiency indices $(0,0)$ and is therefore maximal symmetric.

In fact all self-adjoint operators are maximal symmetric as revealed by the following

Theorem 6 *A closed symmetric operator is self-adjoint if and only if its deficiency indices are $(0,0)$.*

The maximal symmetric operators of particular interest to us are those which have a non-zero deficiency index, since, by theorem 6, they are not self-adjoint.

Example: The maximal symmetric operator $\widehat{P}_+$ has deficiency indices $(1,0)$ and is therefore not self-adjoint. The adjoint of $\widehat{P}_+$ is given by

$$\mathcal{D}(\widehat{P}_+^\dagger) = \left\{ \phi \in L^2(\mathbb{R}^+) : \phi \in AC(\mathbb{R}^+), \phi' \in L^2(\mathbb{R}^+) \right\}$$

and

$$\widehat{P}_+^\dagger \phi = -i\hbar \frac{d\phi}{dx} \quad \forall \phi \in \mathcal{D}(\widehat{P}_+^\dagger),$$

which is clearly a proper extension of $\widehat{P}_+$.

Regarding symmetric operators which have a non-zero deficiency index but which are not closed, we can introduce a notion of essential maximal symmetry analogous to that of essential self-adjointness. Recall, that a symmetric, but not necessarily closed, operator $\widehat{A}$ is said to be essentially self-adjoint if it has a unique self-adjoint extension and that this unique self-adjoint extension coincides with the closure $\overline{A}$ of $\widehat{A}$ [32, pp 129,151], [57, p 256]. An essentially self-adjoint operator has deficiency indices $(0,0)$ and conversely, a symmetric operator with deficiency indices $(0,0)$ is essentially self-adjoint [58, p 231]. This follows from the observation that a (densely defined) operator and its closure share the same adjoint and so possess identical deficiency indices.

The notion of essential self-adjointness is easily extended to one of essential maximal symmetry. If $\widehat{A}$ is a symmetric operator with a zero deficiency index, then, as remarked above, its closure $\overline{A}$ also has a zero deficiency index and is thus maximal symmetric. Now let $\widehat{B}$ be a maximal symmetric extension of $\widehat{A}$. We have,

$$\widehat{B} \supseteq \widehat{A} \Rightarrow \widehat{B}^\dagger \subseteq \widehat{A}^\dagger \Rightarrow (\widehat{B}^\dagger)^\dagger \supseteq (\widehat{A}^\dagger)^\dagger,$$

i.e.

$$\widehat{B} \supseteq \overline{A}$$

as $\widehat{B}$ is closed. So

$$\widehat{B} = \overline{A}$$

since $\overline{A}$ is maximal symmetric. Hence a symmetric operator $\widehat{A}$ which has a zero deficiency index has a unique maximal symmetric extension $\overline{A}$. We may refer to such an $\widehat{A}$ as being essentially maximal symmetric, which generalises the notion of an essentially self-adjoint operator. The operator $\widehat{P}_-^o$ in section 1.5.2 is an example of an essentially maximal symmetric operator that is not maximal symmetric.

Theorem 7 *If a symmetric operator $\widehat{A}$ has equal finite deficiency indices (n, n) then $\widehat{A}$ possesses an n^2 parameter family of self-adjoint extensions.*

Example: The operator $\widehat{P}_o(J)$ has deficiency indices $(1, 1)$ and it has a one parameter family of self-adjoint extensions $\{\widehat{P}^{\lambda}(J) : \lambda \in [0, 2\pi)\}$.

The notion of spectral function of a self-adjoint operator is of central importance in orthodox quantum mechanics, as it is this which allows a probabilistic interpretation through the Born formula. The next section deals with a generalised notion of spectral function which is applicable to symmetric operators.

Generalised Spectral Functions

Definition 8 *A generalised resolution of the identity (GRI) is defined as a one parameter family of bounded operators $\widehat{F}(\lambda)$ which satisfy the following:*

I $\widehat{F}(\infty) = \widehat{I}$,

II $\widehat{F}(-\infty) = \widehat{0}$,

III $\widehat{F}(\lambda - 0) = \widehat{F}(\lambda) \ \ \forall \lambda \in \mathbb{R}$,

IV $\widehat{F}(\lambda_2) - \widehat{F}(\lambda_1)$ *is a positive operator for* $\lambda_1 \leq \lambda_2$,

where all limits are assumed to be strong limits.

If, in addition to satisfying (I) to (IV) above, we also have for every $\lambda_1, \lambda_2 \in \mathbb{R}$

$$\widehat{F}(\lambda_1)\widehat{F}(\lambda_2) = \widehat{F}(\lambda_3) \quad \textit{where } \lambda_3 = min\{\lambda_1, \lambda_2\}$$

then $\widehat{F}(\lambda)$ is called an orthogonal resolution of the identity (ORI).

Definition 9 *A positive-operator-valued (POV) measure is a map $\widehat{F}(\Delta)$ from the σ-field of Borel sets in $\mathbb{R}$ to the bounded operators in a Hilbert space $\mathcal{H}$ which satisfies*

I $\widehat{F}(\mathbb{R}) = \widehat{I}$,

II $\widehat{F}(\emptyset) = \widehat{0}$,

III $\widehat{F}(\cup_i \Delta_i) = \Sigma_i \widehat{F}(\Delta_i) \quad \Delta_i \cap \Delta_j = \emptyset,\ i \neq j$,

IV $\widehat{F}(\Delta)$ *is a positive operator,*

where strong convergence is understood.

If the condition

$$\widehat{F}(\Delta' \cap \Delta'') = \widehat{F}(\Delta')\widehat{F}(\Delta'')$$

is satisfied for every pair of Borel sets (Δ', Δ'') *then* $\widehat{F}(\Delta)$ *is called a projector-valued (PV) measure.*

Theorem 8 *Let* $\widehat{A}$ *be a symmetric operator in a Hilbert space* $\mathcal{H}$ *with a self-adjoint extension* $\widehat{B}^+$ *in a Hilbert space* $\mathcal{H}^+ \supseteq \mathcal{H}$. *Let* $\widehat{P}^+$ *be the projection operator of* $\mathcal{H}^+$ *on* $\mathcal{H}$ *and put*

$$\widehat{F}_\lambda = \widehat{P}^+ \widehat{E}(\widehat{B}^+; \lambda)$$

where $\widehat{E}(\widehat{B}^+; \lambda)$ *is the (unique and orthogonal) spectral function of* $\widehat{B}^+$. *Then for* $\phi \in \mathcal{D}(\widehat{A})$ *and* $\psi \in \mathcal{H}$ *we have*

$$\langle \psi \mid \widehat{A}\phi \rangle = \int_{-\infty}^{\infty} \lambda \, d_\lambda \langle \psi \mid \widehat{F}_\lambda \phi \rangle \tag{1.39}$$

and

$$\left\| \widehat{A}\phi \right\|^2 = \int_{-\infty}^{\infty} \lambda^2 \, d_\lambda \langle \phi \mid \widehat{F}_\lambda \phi \rangle. \tag{1.40}$$

Definition 10 *If* $\widehat{A}$ *is a symmetric operator and* $\widehat{F}(\lambda)$ *is a GRI such that eqns (1.39) and (1.40) hold for all* $\phi \in \mathcal{D}(\widehat{A})$ *and* $\psi \in \mathcal{H}$ *then* $\widehat{F}(\lambda)$ *is called a generalised spectral function of* $\widehat{A}$ *and is denoted* $\widehat{F}(\widehat{A}; \lambda)$. *The POV measure* $\widehat{F}(\widehat{A}; \Delta)$ *defined by* $\widehat{F}(\widehat{A}; \Delta) = \int_\Delta d_\lambda \widehat{F}(\widehat{A}; \lambda)$ *is called the generalised spectral measure of* $\widehat{A}$.

Example: Consider the operator $\widehat{P}_o(J)$. Clearly the spectral function of each self-adjoint extension of $\widehat{P}_o(J)$ is also a generalised spectral function of $\widehat{P}_o(J)$. Note that for such a choice of $\widehat{F}(\widehat{P}_o(J); \lambda)$ we have the proper inclusion

$$\mathcal{D}(\widehat{P}_o(J)) \subset \left\{ \phi : \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{F}(\widehat{P}_o(J); \lambda)\phi \rangle < \infty \right\}.$$

Earlier we saw that $\widehat{P}$ was a type (2) extension of $\widehat{P}_o(J)$. For the generalised spectral function of $\widehat{P}_o(J)$ generated by $\widehat{P}$, i.e.

$$\widehat{F}(\widehat{P}_o(J);\lambda) = \widehat{P}^+\widehat{E}(\widehat{P};\lambda)$$

where $\widehat{P}^+$ is identified with $\widehat{E}(\widehat{X};J)$, we have

$$\mathcal{D}(\widehat{P}_o(J)) = \left\{\phi : \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{F}(\widehat{P}_o(J);\lambda)\phi\rangle < \infty\right\}.$$

Theorem 9 *Every symmetric operator possesses a generalised spectral function.*

Theorem 10 *Every generalised spectral function of a symmetric operator $\widehat{A}$ which is defined in a Hilbert space $\mathcal{H}$ has the form*

$$\widehat{F}(\widehat{A};\lambda) = \widehat{P}^+\widehat{E}(\widehat{B}^+;\lambda),$$

where $\widehat{E}(\widehat{B}^+;\lambda)$ is the spectral function of some self-adjoint extension $\widehat{B}^+$ of the operator $\widehat{A}$, obtained with the aid of an extension of $\mathcal{H}$ to $\mathcal{H}^+ \supseteq \mathcal{H}$, and $\widehat{P}^+$ is the projection operator of $\mathcal{H}^+$ on $\mathcal{H}$.

Clearly for any generalised spectral function of an arbitrary symmetric operator $\widehat{A}$ we have

$$\mathcal{D}(\widehat{A}) \subseteq \left\{\phi : \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{F}(\widehat{A};\lambda)\phi\rangle < \infty\right\}. \tag{1.41}$$

It turns out that the equality in (1.41) holds if and only if $\widehat{B}^+$, of theorem 10, is a type (2) extension. This will be true in particular for maximal symmetric operators as they only possess type (2) extensions. A more important property of maximal symmetric operators is given by the following

Theorem 11 *A closed symmetric operator possesses a unique generalised spectral function if and only if it is maximal. This generalised spectral function is orthogonal if and only if the operator is self-adjoint.*

Note that the generalised spectral function of a maximal symmetric operator is not the generalised spectral function of any other maximal symmetric operator. Since if $\widehat{A}$ and $\widehat{B}$ are maximal symmetric operators with the same (unique) generalised spectral function $\widehat{F}(\lambda)$ then

$$\mathcal{D}(\widehat{A}) = \left\{\phi : \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{F}(\lambda)\phi\rangle < \infty\right\} = \mathcal{D}(\widehat{B})$$

and on this domain,

$$\widehat{A}\phi = \int_{-\infty}^{\infty} \lambda d_\lambda \widehat{F}(\lambda)\phi = \widehat{B}\phi,$$

i.e. $\widehat{A} = \widehat{B}$.

Appendix B: PDFs and GRIs

Suppose we assign to each $\phi \in \mathcal{H}$ a probability distribution function (PDF), $F_\phi(\lambda)$, on $\mathbb{R}$ such that $F_\phi(\lambda) = \langle \phi \mid \widehat{F}(\lambda)\phi \rangle$, where $\widehat{F}(\lambda)$ is a linear operator in $\mathcal{H}$. Then clearly $\widehat{F}(\lambda)$ must be defined *on* $\mathcal{H}$ and thus be bounded. The other properties of $\widehat{F}(\lambda)$ are fixed by the requirement that $F_\phi(\lambda)$ is a PDF for every $\phi \in \mathcal{H}$.

A function $F : \mathbb{R} \longrightarrow \mathbb{R}$ is a PDF on $\mathbb{R}$ if and only if [60]:

1a. $F(\infty) = 1$.

2a. $F(-\infty) = 0$.

3a. $F(\lambda - 0) = F(\lambda) \;\; \forall \lambda \in \mathbb{R}$.

4a. $F(\lambda_1) \leq F(\lambda_2)$ wherever $\lambda_1 \leq \lambda_2$.

So, if $F_\phi(\lambda)$ is a PDF on $\mathbb{R}$ for every $\phi \in \mathcal{H}$ then (1a) to (4a) above respectively imply the following:

1b. $\widehat{F}(\infty) = \widehat{I}$.

2b. $\widehat{F}(-\infty) = \widehat{0}$.

3b. $\widehat{F}(\lambda - 0) = \widehat{F}(\lambda) \;\; \forall \lambda \in \mathbb{R}$.

4b. $\widehat{F}(\lambda_2) - \widehat{F}(\lambda_1)$ is a positive operator wherever $\lambda_1 \leq \lambda_2$.

That (1b), (2b) and (3b) hold in the strong operator topology is a corollary of the following

Lemma 2 *If $\{\widehat{A}_t\}$ is a sequence of bounded operators which converges ultraweakly to the bounded operator $\widehat{A}$, i.e.*

$$\lim_{t\to\infty} \langle \phi \mid (\widehat{A} - \widehat{A}_t)\phi\rangle = 0 \quad \forall \phi \in \mathcal{H},$$

such that either

$$(a) \qquad 0 \leq \langle \phi \mid \widehat{A}_t\phi\rangle \leq \langle \phi \mid \widehat{A}\phi\rangle \leq 1 \quad \forall t \in \boldsymbol{R}, \phi \in \mathcal{H}$$

or

$$(b) \qquad 0 \leq \langle \phi \mid \widehat{A}\phi\rangle \leq \langle \phi \mid \widehat{A}_t\phi\rangle \leq 1 \quad \forall t \in \boldsymbol{R}, \phi \in \mathcal{H},$$

then $\{\widehat{A}_t\}$ converges strongly to $\widehat{A}$.

Proof: Assume $\{\widehat{A}_t\}$ is a sequence of type (a), so that $\widehat{A} - \widehat{A}_t$ is a positive operator. The generalised Schwartz inequality [61, p 262] gives

$$\left\|(\widehat{A} - \widehat{A}_t)\phi\right\|^4 \leq \langle \phi \mid (\widehat{A} - \widehat{A}_t)\phi\rangle\langle(\widehat{A} - \widehat{A}_t)\phi \mid (\widehat{A} - \widehat{A}_t)(\widehat{A} - \widehat{A}_t)\phi\rangle,$$

and since

$$\langle \psi \mid (\widehat{A} - \widehat{A}_t)\psi\rangle \leq 1 \quad \forall \psi \in \mathcal{H}$$

then

$$\left\|(\widehat{A} - \widehat{A}_t)\phi\right\|^4 \leq \langle \phi \mid (\widehat{A} - \widehat{A}_t)\phi\rangle.$$

Thus

$$\lim_{t\to\infty} \left\|(\widehat{A} - \widehat{A}_t)\phi\right\| = 0.$$

For a sequence of type (b) we can apply the generalised Schwartz inequality to $\widehat{A}_t - \widehat{A}$ and the desired result follows, cf. [28, pp 14–15].

Clearly $\widehat{F}(\lambda)$ is a generalised resolution of the identity (GRI) for $\mathcal{H}$.

Appendix C: The Radial Momentum Operator and its Generalised Spectral Function

In spherical polar coordinates, $L^2(\mathbb{R}^3, d\mathbf{r})$ has the decomposition [62, p 151]:

$$L^2(\mathbb{R}^3, d\mathbf{r}) = L^2(\mathbb{R}^+, r^2 dr) \otimes L^2(S^2, \sin\theta d\theta d\varphi).$$

Let $\widehat{I}$ denote the identity operator on $L^2(S^2, \sin\theta d\theta d\varphi)$, then the radial momentum operator $\widehat{p}_r = -i\hbar(1/r)(\partial/\partial r)r$ is identified with the closure of the operator $\widehat{P}_r \otimes \widehat{I}$ defined on $D(\widehat{P}_r) \otimes L^2(S^2, \sin\theta d\theta d\varphi)$ where

$$D(\widehat{P}_r) = \{\phi \in L^2(\mathbb{R}^+, r^2 dr) : \phi \in AC(\mathbb{R}^+), \frac{1}{r}\frac{d}{dr}r\phi \in L^2(\mathbb{R}^+, r^2 dr) \text{ and } \lim_{r\to 0} r|\phi(r)| = 0\}$$

and for each $\phi \in D(\widehat{P}_r)$,

$$\widehat{P}_r\phi = -i\hbar\frac{1}{r}\frac{d}{dr}r\phi.$$

Now $\widehat{P}_r$ is maximal symmetric in $L^2(\mathbb{R}^+, r^2 dr)$ but not self-adjoint [32, pp 139–141,157]. Note that $\widehat{P}_r$ here corresponds to $\widehat{A}_k^*$, $k = 2$, in [32].

Next consider the operator $\widehat{P}_+$ defined in $L^2(\mathbb{R}^+, dr)$ on domain

$$D(\widehat{P}_+) = \{\phi_+ \in L^2(\mathbb{R}^+, dr) : \phi_+ \in AC(\mathbb{R}^+), \frac{d\phi_+}{dr} \in L^2(\mathbb{R}^+, dr) \text{ and } \lim_{r\to 0} |\phi_+(r)| = 0\}$$

by

$$\widehat{P}_+\phi_+ = -i\hbar\frac{d\phi_+}{dr}$$

where $\widehat{P}_+$ is also maximal symmetric but not self-adjoint (appendix A). There is a unitary map, $\widehat{U}$, between $L^2(\mathbb{R}^+, r^2 dr)$ and $L^2(\mathbb{R}^+, dr)$ defined by

$$\widehat{U}\phi = r\phi \in L^2(\mathbb{R}^+, dr) \qquad \forall \phi \in L^2(\mathbb{R}^+, r^2 dr)$$

and

$$\widehat{U}^{-1}\phi_+ = \frac{\phi_+}{r} \in L^2(\mathbb{R}^+, r^2 dr) \qquad \forall \phi_+ \in L^2(\mathbb{R}^+, dr).$$

Clearly $\widehat{P}_r$ and $\widehat{P}_+$ are unitarily equivalent, i.e.

$$\widehat{P}_r = \widehat{U}^{-1}\widehat{P}_+\widehat{U}; \quad \widehat{P}_+ = \widehat{U}\widehat{P}_r\widehat{U}^{-1}.$$

The operator $\widehat{P}_+$, being maximal symmetric, possesses a unique generalised spectral function $\widehat{F}(\widehat{P}_+;\lambda)$. One can easily verify that the generalised spectral function for $\widehat{P}_r$, $\widehat{F}(\widehat{P}_r;\lambda)$, is $\widehat{U}^{-1}\widehat{F}(\widehat{P}_+;\lambda)\widehat{U}$ and that the generalised spectral function for $\widehat{p}_r$, $\widehat{F}(\widehat{p}_r;\lambda)$, is then just $\overline{\widehat{F}(\widehat{P}_r;\lambda)\otimes\widehat{I}}$. We need now only to find an explicit expression for $\widehat{F}(\widehat{P}_r;\lambda)$.

Let $\widehat{E}(\widehat{X};\lambda)$ and $\widehat{E}(\widehat{P};\lambda)$ denote the respective (standard) spectral functions of the familiar position and momentum operators in $L^2(\mathbb{R}, dr)$, i.e. for each $\phi \in L^2(\mathbb{R}, dr)$,

$$\left(\widehat{E}(\widehat{X};\lambda)\phi\right)(r) = \chi_{(-\infty,\lambda]}(r)\phi(r)$$

and

$$\left(\widehat{E}(\widehat{P};\lambda)\phi\right)(r) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\lambda} d\lambda' \int_{-\infty}^{\infty} dr' e^{\frac{i}{\hbar}\lambda'(r-r')}\phi(r').$$

Now since $L^2(\mathbb{R}, dr) \supset L^2(\mathbb{R}^+, dr)$ and $\widehat{P}$ is a generalised self-adjoint extension of $\widehat{P}_+$ [11, pp 138–139], then for each $\phi_+ \in L^2(\mathbb{R}^+, dr)$ we have [25, pp 63–64], [11, pp 128–130]:

$$\begin{aligned} \left(\widehat{F}(\widehat{P}_+,\lambda)\phi_+\right)(r) &= \chi_{[0,\infty)}(r)\left(\widehat{E}(\widehat{P};\lambda)\phi_+\right)(r) \qquad (1.42) \\ &= \chi_{[0,\infty)}(r)\frac{1}{2\pi\hbar}\int_{-\infty}^{\lambda} d\lambda' \int_{-\infty}^{\infty} dr' e^{\frac{i}{\hbar}\lambda'(r-r')}\phi_+(r'). \end{aligned}$$

Thus

$$\left(\widehat{F}(\widehat{P}_r;\lambda)\phi\right)(r) = \frac{1}{2\pi\hbar r}\int_{-\infty}^{\lambda} d\lambda' \int_{0}^{\infty} dr' e^{\frac{i}{\hbar}\lambda'(r-r')} r'\phi(r')$$

$\forall \phi \in L^2(\mathbb{R}^+, r^2 dr)$.

Appendix D: Feynman's Derivation of Josephson's Equation

A wavefunction is associated with each side of a Josephson junction which separates two superconductors (figure 1.3), ϕ_- with the left side and ϕ_+ with the right side, and these are assumed to be related by the equations [49]

$$i\hbar\frac{\partial\phi_-}{\partial t} = U_-\phi_- + K\phi_+ \tag{1.43}$$

$$i\hbar\frac{\partial\phi_+}{\partial t} = U_+\phi_+ + K\phi_-. \tag{1.44}$$

The coupling constant K, which is a characteristic of the junction, allows the possibility of a current to flow across the junction.

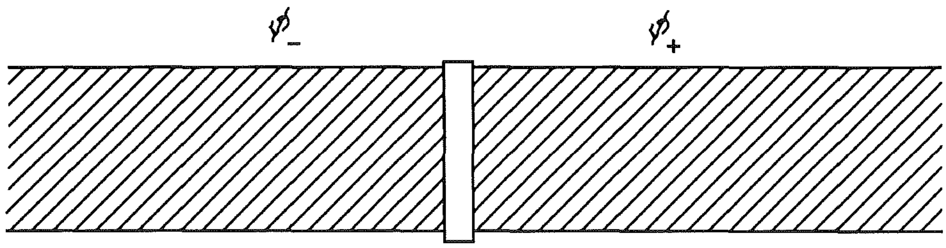

Figure 1.3: Superconductor Containing a Josephson Junction

We substitute into eqns (1.43) and (1.44),

$$\phi_- = \sqrt{\rho_-}e^{i\lambda_-}$$

and

$$\phi_+ = \sqrt{\rho_+}e^{i\lambda_+},$$

where ρ_-, ρ_+ are the electron number densities on each side of the junction and λ_-, λ_+ are the respective phases. The following equations are obtained:

$$\hbar\frac{\partial\rho_-}{\partial t} = 2K\sqrt{\rho_-\rho_+}\sin(\lambda_+ - \lambda_-) \tag{1.45}$$

$$\hbar\frac{\partial\rho_+}{\partial t} = -2K\sqrt{\rho_-\rho_+}\sin(\lambda_+ - \lambda_-). \tag{1.46}$$

Equations (1.45) and (1.46) are then assumed to describe a current flowing through the junction. The 'left to right current' is thus

$$J = \frac{\partial\rho_-}{\partial t} = -\frac{\partial\rho_+}{\partial t} = \frac{2K\sqrt{\rho_-\rho_+}}{\hbar}\sin(\lambda_+ - \lambda_-) \tag{1.47}$$

or

$$J = J_o \sin\lambda \tag{1.48}$$

where $J_o = 2K\sqrt{\rho_-\rho_+}/\hbar$ and $\lambda = \lambda_+ - \lambda_-$.

Note that if J is to be a constant steady supercurrent then both ρ_- and ρ_+ should be time independent. Clearly though, this is not the case. By eqn (1.47), ρ_+ (ρ_-) increases linearly with time while ρ_- (ρ_+) decreases linearly with time. To overcome this problem, one assumes that the two sides of the junction are connected to a battery so that there is a potential across the junction. This will ensure that ρ_- and ρ_+ are maintained at constant values [49].

In our approach (section 1.5.2) the Josephson effect arises in a significantly less ad hoc manner than in that above. In particular, we do not need to assume the existence of a potential across the junction in order to establish a steady current. Essentially, all that we require is that the state of the system, i.e. the state of the quasi-particle representing the condensate, is a simultaneous eigenfunction of a current operator and a Hamiltonian operator.

Appendix E: Supercurrent Operators and Self-Adjoint Extensions

Denote the sets $(-\infty, 0)$ and $(0, \infty)$ by $\mathbb{R}_o^-$ and $\mathbb{R}_o^+$ respectively. Define the operator $\widehat{P}_-$ by

$$\mathcal{D}(\widehat{P}_-) = \left\{\phi \in L^2(\mathbb{R}_o^-) : \phi \in AC(\mathbb{R}_o^-), \phi' \in L^2(\mathbb{R}_o^-), \phi(0^-) = 0\right\}$$

$$\widehat{P}_-\phi = -i\hbar\frac{d\phi}{dx} \quad \forall\phi \in \mathcal{D}(\widehat{P}_-),$$

where $\widehat{P}_-$ is maximal symmetric with deficiency indices $(0, 1)$.

Similarly, we define the operator $\widehat{P}_+$ by

$$\mathcal{D}(\widehat{P}_+) = \left\{\phi \in L^2(\mathbb{R}_o^+) : \phi \in AC(\mathbb{R}_o^+), \phi' \in L^2(\mathbb{R}_o^+), \phi(0^+) = 0\right\}$$

$$\widehat{P}_+\phi = -i\hbar\frac{d\phi}{dx} \quad \forall\phi \in \mathcal{D}(\widehat{P}_+),$$

where $\widehat{P}_+$ is also maximal symmetric, its deficiency indices being $(1, 0)$.

It is known [42, pp 140,145,149] that $\widehat{P}^o \equiv \widehat{P}_- \oplus \widehat{P}_+$ is a closed symmetric operator with deficiency indices $(1, 1)$; it therefore possesses a one parameter family of self-adjoint extensions, which we shall denote by $\{\widehat{P}_\lambda : \lambda \in \mathbb{R}\}$.

Proposition: *The self-adjoint extension corresponding to a particular λ is given by*

$$\begin{aligned}\mathcal{D}(\widehat{P}_\lambda) = \{\phi = \phi_- \oplus \phi_+ \in L^2(\mathbb{R}_o^-) \oplus L^2(\mathbb{R}_o^+) : \phi_\pm &\in AC(\mathbb{R}_o^\pm), \\ \phi'_\pm &\in L^2(\mathbb{R}_o^\pm), \phi_-(0^-) = e^{-i\lambda}\phi_+(0^+)\}\end{aligned}$$

and

$$\widehat{P}_\lambda \phi = -i\hbar(\phi'_- \oplus \phi'_+) \quad \forall \phi \in \mathcal{D}(\widehat{P}_\lambda).$$

Proof: This proof closely follows that for the 'particle in a box' problem in [50, pp 141–142].

Let $\widehat{\mathcal{P}}^o$ be a symmetric extension of $\widehat{P}^o$, i.e.

$$\widehat{P}^o \subseteq \widehat{\mathcal{P}}^o \subseteq (\widehat{\mathcal{P}}^o)^\dagger \subseteq (\widehat{P}^o)^\dagger. \tag{1.49}$$

Now $(\widehat{P}^o)^\dagger$ is given by [42, pp 140,145]

$$\mathcal{D}\left((\widehat{P}^o)^\dagger\right) = \mathcal{D}(\widehat{P}^\dagger_-) \oplus \mathcal{D}(\widehat{P}^\dagger_+),$$

$$(\widehat{P}^o)^\dagger \phi = \widehat{P}^\dagger_- \phi_- \oplus \widehat{P}^\dagger_+ \phi_+ \quad \forall \phi = \phi_- \oplus \phi_+ \in \mathcal{D}\left((\widehat{P}^o)^\dagger\right),$$

where $\widehat{P}^\dagger_-$ is defined by

$$\mathcal{D}(\widehat{P}^\dagger_-) = \left\{\phi \in L^2(\mathbb{R}^-_o) : \phi \in AC(\mathbb{R}^-_o), \phi' \in L^2(\mathbb{R}^-_o)\right\},$$

$$\widehat{P}^\dagger_- \phi = -i\hbar \frac{d\phi}{dx} \quad \forall \phi \in \mathcal{D}(\widehat{P}^\dagger_-)$$

and $\widehat{P}^\dagger_+$ is similarly defined in $L^2(\mathbb{R}^+_o)$.

So, if $\phi = \phi_- \oplus \phi_+ \in \mathcal{D}\left((\widehat{P}^o)^\dagger\right)$ then, by (1.49), $\phi_\pm \in AC(\mathbb{R}^\pm_o)$ and both $\widehat{\mathcal{P}}^o$ and $(\widehat{\mathcal{P}}^o)^\dagger$ have the formal expression $\widehat{\mathcal{P}}^o_- \oplus \widehat{\mathcal{P}}^o_+$ where $\widehat{\mathcal{P}}^o_-$ and $\widehat{\mathcal{P}}^o_+$ act as $-i\hbar d/dx$.

For $\phi \in \mathcal{D}(\widehat{\mathcal{P}}^o)$ and $\psi \in \mathcal{D}\left((\widehat{\mathcal{P}}^o)^\dagger\right)$ we have

$$\langle \widehat{\mathcal{P}}^o \phi \mid \psi \rangle - \langle \phi \mid (\widehat{\mathcal{P}}^o)^\dagger \psi \rangle = 0$$

$$\Longrightarrow \qquad \langle \widehat{\mathcal{P}}^o_- \phi_- \mid \psi_- \rangle_- + \langle \widehat{\mathcal{P}}^o_+ \phi_+ \mid \psi_+ \rangle_+$$

$$- \langle \phi_- \mid (\widehat{\mathcal{P}}^o_-)^\dagger \psi_- \rangle_- - \langle \phi_+ \mid (\widehat{\mathcal{P}}^o_+)^\dagger \psi_+ \rangle_+ = 0 \tag{1.50}$$

where

$$\langle \phi_- \mid \psi_- \rangle_- = \int_{-\infty}^0 \phi^*_-(x)\psi_-(x)dx, \qquad \langle \phi_+ \mid \psi_+ \rangle_+ = \int_0^\infty \phi^*_+(x)\psi_+(x)dx.$$

Since $\phi_-, \psi_- \in AC(\boldsymbol{R}_o^-)$ and $\phi_+, \psi_+ \in AC(\boldsymbol{R}_o^+)$ then, integrating by parts in the usual manner, eqn (1.50) can be reduced to

$$\phi_-^*(0^-)\psi_-(0^-) - \phi_+^*(0^+)\psi_+(0^+) = 0. \tag{1.51}$$

Now suppose $\widehat{\mathcal{P}}^o$ is self-adjoint and let $\phi = \phi_- \oplus \phi_+ \in \{\mathcal{D}(\widehat{\mathcal{P}}^o) - \mathcal{D}(\widehat{P}^o)\}$. Equation (1.51) requires $|\phi_-(0^-)|^2 = |\phi_+(0^+)|^2$ and since $\phi \notin \mathcal{D}(\widehat{P}^o)$ then $\phi_-(0^-) \neq 0 \neq \phi_+(0^+)$, so there is a $\lambda \in \boldsymbol{R}$ such that $\phi_-(0^-) = e^{-i\lambda}\phi_+(0^+)$.

If $\psi \equiv \psi_- \oplus \psi_+$ is any other function in $\mathcal{D}(\widehat{\mathcal{P}}^o)$ then substituting $\phi_-(0^-) = e^{-i\lambda}\phi_+(0^+)$ into eqn (1.51) yields

$$e^{i\lambda}\phi_+^*(0^+)\psi_-(0^-) - \phi_+^*(0^+)\psi_+(0^+) = 0$$

and since $\phi \notin \mathcal{D}(\widehat{P}^o)$ then $\phi_-(0^-) \neq 0 \neq \phi_+(0^+)$ so $\psi_-(0^-) = e^{-i\lambda}\psi_+(0^+)$ and it follows that for some λ,

$$\begin{aligned}\mathcal{D}(\widehat{\mathcal{P}}^o) = \{\phi = \phi_- \oplus \phi_+ \in L^2(\boldsymbol{R}_o^-) \oplus L^2(\boldsymbol{R}_o^+) : \phi_\pm &\in AC(\boldsymbol{R}_o^\pm), \\ \phi'_\pm &\in L^2(\boldsymbol{R}_o^\pm), \phi_-(0^-) = e^{-i\lambda}\phi_+(0^+)\}\end{aligned}$$

and

$$\widehat{\mathcal{P}}^o\phi = -i\hbar(\phi'_- \oplus \phi'_+) \quad \forall\phi \in \mathcal{D}(\widehat{\mathcal{P}}^o).$$

Let $\widehat{\mathcal{P}}^o_\lambda$ be defined like $\widehat{\mathcal{P}}^o$ except that λ is now arbitrary. Clearly $\widehat{\mathcal{P}}^o_\lambda$ is symmetric and an extension of $\widehat{P}^o$.

For $\phi \in \mathcal{D}(\widehat{\mathcal{P}}^o_\lambda)$ and $\psi \in \mathcal{D}\left((\widehat{\mathcal{P}}^o_\lambda)^\dagger\right)$, we again arrive at eqn (1.51), which requires $\psi_-(0^-) = e^{-i\lambda}\psi_+(0^+)$, so that $\psi \in \mathcal{D}(\widehat{\mathcal{P}}^o_\lambda)$ and it follows that $\widehat{\mathcal{P}}^o_\lambda$ is self-adjoint for every $\lambda \in \boldsymbol{R}$. Thus

$$\{\widehat{P}_\lambda : \lambda \in \boldsymbol{R}\} = \{\widehat{\mathcal{P}}^o_\lambda : \lambda \in \boldsymbol{R}\} = \{\widehat{\mathcal{P}}^o_\lambda : \lambda \in (-\pi, \pi]\}.$$

From section 1.5.2, we have $\widehat{J}^o = (e/\pi m)\widehat{P}^o$ and so the family $\{\widehat{J}_\lambda : \lambda \in (-\pi, \pi]\}$, where $\widehat{J}_\lambda = (e/\pi m)\widehat{P}_\lambda$, constitutes the family of supercurrent operators for the system comprising two semi-infinite one-dimensional superconductors separated by a Josephson junction.

Appendix F: Boundary Conditions for Self-Adjoint Extensions of $\widehat{H}^O$

Our aim here is to find all the self-adjoint extensions of the operator $\widehat{H}^o$ from section 1.5.2 and to show that each of these extensions can be characterised by a boundary condition at the junction. We shall do this by following the treatment of Exner and Šeba [53].

Define Δ_o by $\Delta_o = (2m/\hbar^2)\overline{\widehat{H}^o}$ where $\overline{\widehat{H}^o}$ is the closure of $\widehat{H}^o$. We have ([42, p 145],[58, pp 160,162]):

$$\overline{\widehat{H}^o} = \overline{\widehat{H}^o_-} \oplus \overline{\widehat{H}^o_+}$$

with

$$\mathcal{D}(\overline{\widehat{H}^o_\pm}) = \{\psi \in \mathcal{H}_\pm : \psi \in A_2(\mathbb{R}_o^\pm), \psi'' \in \mathcal{H}_\pm, \psi(0^\pm) = \psi'(0^\pm) = 0\}$$

and

$$\overline{\widehat{H}^o_\pm}\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \qquad \forall\psi \in \mathcal{D}(\overline{\widehat{H}^o_\pm})$$

where $A_2(\boldsymbol{R}_o^\pm)$ denotes the set of continuously differentiable functions on $\boldsymbol{R}_o^\pm$ which have absolutely continuous first derivatives.

Let N_+ and N_- be the deficiency spaces of Δ_o, i.e.

$$N_+ = \left\{\phi \in \mathcal{D}(\Delta_o^\dagger) : (\Delta_o^\dagger - i)\phi = 0\right\}, \qquad N_- = \left\{\phi \in \mathcal{D}(\Delta_o^\dagger) : (\Delta_o^\dagger + i)\phi = 0\right\}$$

and let Δ_s be a self-adjoint extension of Δ_o. The second formula of von Neumann [58, p 238] tells us that there is a unitary mapping $\widehat{V}$ of N_+ onto N_- such that

$$\mathcal{D}(\Delta_s) = \mathcal{D}(\Delta_o) + \left\{\varphi + \widehat{V}\varphi : \varphi \in N_+\right\}$$

and on $\mathcal{D}(\Delta_s)$,

$$\Delta_s\Phi = \Delta_o\phi + i\varphi - i\widehat{V}\varphi$$

where

$$\Phi = \phi + \varphi + \widehat{V}\varphi; \qquad \phi \in \mathcal{D}(\Delta_o),\ \varphi \in N_+.$$

The space N_+ is two-dimensional and possesses normalised basis functions

$$g_1 = g_- \oplus 0, \qquad g_2 = 0 \oplus g_+,$$

with

$$g_- = \gamma e^{\rho x} \in \mathcal{H}_-, \qquad g_+ = \gamma e^{-\rho x} \in \mathcal{H}_+$$

where $\rho = exp(-i\pi/4)$ and γ is a normalisation constant. Likewise for N_- we have normalised basis functions

$$f_1 = f_- \oplus 0, \qquad f_2 = 0 \oplus f_+,$$

with

$$f_- = \gamma e^{\rho^* x} \in \mathcal{H}_-, \qquad f_+ = \gamma e^{-\rho^* x} \in \mathcal{H}_+$$

where $\rho^* = exp(i\pi/4)$. Now let

$$\varphi = \sum_{k=1}^{2} \alpha_k g_k, \qquad \widehat{V} g_k = \sum_{j=1}^{2} u_{jk} f_j,$$

so that

$$\Phi = \phi + \sum_{k=1}^{2} \alpha_k \left(g_k + \sum_{j=1}^{2} u_{jk} f_j \right).$$

Now since (u_{jk}) is a 2×2 unitary matrix than we have a four-(real)-parameter family of self-adjoint extensions. This can be reduced to a two-parameter family by symmetry considerations. We have assumed dynamical symmetry of the superconducting system about the junction. This means that the effect of the junction on a supercurrent flowing left to right is the same as that on a supercurrent flowing right to left. Since the dynamics are governed by the Hamiltonians, then Δ_s, and consequently $\widehat{V}$, should be invariant with respect to the interchange of g_1, f_1 and g_2, f_2. It follows that we have

$$u_{11} = u_{22} \equiv u, \qquad u_{12} = u_{21} \equiv v$$

or

$$u_{jk} = u\delta_{jk} + v(1 - \delta_{jk}).$$

Next we shall show that each of the self-adjoint extensions, as specified by a unitary matrix (u_{jk}), can be identified with a corresponding boundary condition at the junction. Firstly, we note that each $\Phi \in \mathcal{D}(\Delta_s)$ is of the form $\Phi = \Phi_1 + \Phi_2$ where

$$\Phi_1 = \phi_1 + \alpha_1 g_1 + (\alpha_1 u + \alpha_2 v) f_1, \qquad \Phi_2 = \phi_2 + \alpha_2 g_2 + (\alpha_1 v + \alpha_2 u) f_2 \tag{1.52}$$

with

$$\phi_1 = \phi_- \oplus 0, \;\; \phi_- \in \mathcal{D}(\overline{\widehat{H}^o_-}); \qquad \phi_2 = 0 \oplus \phi_+, \;\; \phi_+ \in \mathcal{D}(\overline{\widehat{H}^o_+}).$$

We then *choose* boundary conditions

$$\Phi_{10} = -a\Phi'_{10} + b\Phi'_{20} \tag{1.53}$$

$$\Phi_{20} = a\Phi'_{20} - b\Phi'_{10} \tag{1.54}$$

where a dash signifies a derivative with respect to x and a subscript 0 denotes the function evaluated at the junction. Substituting (1.52) into (1.53) or (1.54) and equating the coefficients of the arbitrary constants α_1,α_2 yields

$$1 + u = -a(\rho + \rho^* u) - b\rho^* v \tag{1.55}$$

$$v = -a\rho^* v - b(\rho + \rho^* u). \tag{1.56}$$

Provided the denominators are non-zero, we have

$$a = \frac{\rho^* v^2 - (1+u)(\rho + \rho^* u)}{(\rho + \rho^* u)^2 - (\rho^* v)^2}, \qquad b = \frac{(\rho^* - \rho)v}{(\rho + \rho^* u)^2 - (\rho^* v)^2} \tag{1.57}$$

$$u = \frac{b^2 - a^2 - a(\rho + \rho^*) - 1}{(1 + a\rho^*)^2 - (b\rho^*)^2}, \qquad v = \frac{(\rho^* - \rho)b}{(1 + a\rho^*)^2 - (b\rho^*)^2}. \tag{1.58}$$

Using the unitarity conditions

$$|u|^2 + |v|^2 = 1 \text{ and } uv^* + vu^* = 0,$$

the parameters a, b as given by (1.57) can be shown to be real. One can also show that $(1+a\rho^*)^2 - (b\rho^*)^2 = 0$ is not satisfied for any real a, b. So every $a, b \in \mathbb{R}$ determines a u, v and hence a self-adjoint extension and every pair u, v which does not satisfy $(\rho + \rho^* u)^2 - (\rho^* v)^2 = 0$ determines real parameters a, b which in turn identify a particular boundary condition at the junction.

For the case $\rho + \rho^* u = \rho^* v$, i.e. $u = i + v$, we try the following boundary conditions:

$$\Phi'_{10} + \Phi'_{20} = 0 \tag{1.59}$$

$$\Phi_{10} + \Phi_{20} = c(\Phi'_{20} - \Phi'_{10}). \tag{1.60}$$

Substituting (1.52) into (1.59) and (1.60) and equating the coefficients of the arbitrary constants α_1, α_2 we get $\rho + \rho^* u = \rho^* v$, as required. Provided $v \neq 0$, we have, by eqn (1.60),

$$c = \frac{(i-1)v - 1}{\sqrt{2}v}.$$

Using the unitarity conditions, which, for $u = i + v$, reduce to the single equation

$$|v|^2 + \frac{1}{2}(v^* - v)i = 0,$$

one can show that c is real. We also have

$$v = \frac{1}{i - 1 - \sqrt{2}c},$$

which is defined for all $c \in \mathbb{R}$.

For the case $\rho + \rho^* u = -\rho^* v$, i.e. $u = i - v$, we try the following boundary conditions:

$$\Phi'_{10} - \Phi'_{20} = 0 \tag{1.61}$$

$$\Phi_{10} - \Phi_{20} = d\Phi'_{10} \tag{1.62}$$

Substituting (1.52) into (1.61) and (1.62) and equating the coefficients of the arbitrary constants α_1, α_2 we get $\rho + \rho^* u = -\rho^* v$, as required. If $v \neq 0$, then we can use eqn (1.62) to express d in terms of v. We have

$$d = \sqrt{2}\frac{(1-i)v-1}{v}.$$

For $u = i - v$, the unitarity conditions are reduced to the equation

$$|v|^2 + \frac{1}{2}(v - v^*)i = 0$$

and by using this, d can be shown to be real. We also have,

$$v = \frac{\sqrt{2}}{\sqrt{2} - i\sqrt{2} - d},$$

which is defined for all $d \in \mathbb{R}$.

Finally, for the case $v = 0$ and $\rho + \rho^* u = 0$, i.e. $v = 0, u = i$, the unitarity conditions are satisfied automatically and the appropriate boundary condition is

$$\Phi'_{10} = \Phi'_{20} = 0. \tag{1.63}$$

To verify this we substitute (1.52) into (1.63) and equate the coefficients of the arbitrary constants α_1, α_2 to get $v = 0$ and $\rho + \rho^* u = 0$, as required.

We have now covered all possible u and v and have thus shown that each self-adjoint extension, as determined by a particular unitary map $\widehat{V}$, can be characterised by a boundary condition at the junction. In section 1.5.2 we have incorporated boundary condition (1.63) into boundary conditions (1.61) and (1.62) by formally extending the range of d to $\mathbb{R} \cup \{\infty\}$.

Chapter 2

ADAPTED OBSERVABLES

In chapter 1 the set of ideal observables was identified with the set of maximal symmetric operators. Such observables are defined irrespective of how they are measured. We saw how the notion of approximate observable was useful in describing the non-ideal measurement of observables due to the finite resolution of the measuring device (MD).

In this chapter we consider other aspects of measurement which warrant a description in terms of *adapted observables*, which are obtained from the (ideal) observables by a particular process which will depend on the nature of the measurement. For example, the approximate observables of chapter 1 are obtained from the original ideal observable by a randomisation process involving a confidence function which reflects the finite resolution of the MD.

2.1 Unsharpness and Closely Related Families of Observables

We have already seen in chapter 1 how a measurement of an observable made with an MD of limited resolution may be described in terms of a non-orthogonal GRI. The position observable which was used to illustrate this is especially relevant as it has a continuous spectrum. We wish now to demonstrate how a similar situation can arise even when we are dealing with observables which possess purely discrete spectra.

The fact that an MD has a finite resolution means that it may well be impossible to distinguish a related set of maximal symmetric operators. This is best illustrated with an example. Consider the family of momentum observables for a particle confined to an interval J of finite length L. This is represented by the family of self-adjoint operators $\{\widehat{P}^\lambda(J) : \lambda \in (-\pi, \pi]\}$ from appendix A. Each $\widehat{P}^\lambda(J)$ has eigenfunctions ϕ_n^λ and eigenvalues P_n^λ, where $n = 0, \pm 1, \pm 2, ...$ and

$$\phi_n^\lambda(x) = \frac{1}{\sqrt{L}} e^{iP_n^\lambda x}, \qquad P_n^\lambda = (2\pi n + \lambda)\frac{\hbar}{L}.$$

To pick out a particular $\widehat{P}^\lambda(J)$ we may, say, try to obtain its eigenvalues by measurement since these are unique to $\widehat{P}^\lambda(J)$. But this is generally impossible with an MD of finite resolution since the eigenvalues of $\widehat{P}^\lambda(J)$ will, for some $\lambda' \neq \lambda$, lie too close to those of $\widehat{P}^{\lambda'}(J)$ to be distinguished. In a recent paper [29] operators like $\widehat{P}^\lambda(J)$ are utilised to model superconducting ring devices with a Josephson junction; the parameter λ is seen there to be determined by an externally applied magnetic field. As λ is continuous then a confidence function should be introduced to establish realistic PDFs for describing the values recorded by the MD.

Since the family $\{\widehat{P}^\lambda(J) : \lambda \in (-\pi, \pi]\}$ constitutes the set of self-adjoint extensions of the symmetric operator $\widehat{P}_o(J)$ (appendix A), we have here an example of a symmetric operator associated with a family of observables (cf. section 1.3.3).

Let $\phi \in \mathcal{D}(\widehat{P}_o(J))$, then for every $\lambda \in (-\pi, \pi]$, we have

$$\langle \phi \mid \widehat{P}_o(J)\phi \rangle = \int_{-\infty}^{\infty} \alpha d_\alpha \langle \phi \mid \widehat{E}(\widehat{P}^\lambda(J); \alpha)\phi \rangle$$

and

$$\left\| \widehat{P}_o(J)\phi \right\|^2 = \int_{-\infty}^{\infty} \alpha^2 d_\alpha \langle \phi \mid \widehat{E}(\widehat{P}^\lambda(J); \alpha)\phi \rangle.$$

For a given $\lambda \in (-\pi, \pi]$ the spectral function $\widehat{E}(\widehat{P}^\lambda(J); \alpha)$ is defined, in Dirac's Bra-Ket notation, by

$$\widehat{E}(\widehat{P}^\lambda(J); \alpha) = \sum_{n=-\infty}^{N} |\phi_n^\lambda\rangle\langle\phi_n^\lambda|$$

where

$$(2\pi N + \lambda)\frac{\hbar}{L} \leq \alpha < (2\pi(N+1) + \lambda)\frac{\hbar}{L},$$

and we have

$$\begin{aligned}\widehat{P}^{\lambda}(J) &= \sum_{n=-\infty}^{\infty} P_n^{\lambda}|\phi_n^{\lambda}\rangle\langle\phi_n^{\lambda}| \\ &= \int_{-\infty}^{\infty} \alpha d_{\alpha}\widehat{E}(\widehat{P}^{\lambda}(J);\alpha).\end{aligned}$$

Suppose that we desire to measure observable $\widehat{P}^{\lambda_o}(J)$. For sake of clarity, we shall assume $\lambda_o = 0$.[1] There is no loss of generality in doing this since for non-zero λ_o, the parameter λ can take values from the interval $(-\pi + \lambda_o, \pi + \lambda_o]$ as any interval of length 2π will suffice.

Introduce a confidence function $g(\lambda)$ defined on $(-\pi, \pi]$, i.e. $g(\lambda)$ is a probability density function peaked at, and symmetric about, $\lambda = 0$. We assume the variance $\mathcal{V}(g)$ satisfies

$$\mathcal{V}(g) << 4\pi^2,$$

i.e. $(\hbar/L)^2\mathcal{V}(g)$ is much less than the spacing between the eigenvalues of each observable $\widehat{P}^{\lambda}(J)$. This condition ensures that all uncertainty in a nominal value $P_n^{\lambda_o}$ can be associated with λ_o.

Ideally, the probability that a measurement of observable $\widehat{P}^{\lambda_o}(J)$ will return a value of $P_n^{\lambda_o}$, for a given state $\phi \in \mathcal{D}(\widehat{P}_o(J))$, is

$$f_{\phi}^{\lambda_o}(n) \equiv \langle\phi \mid \widehat{P}_n^{\lambda_o}\phi\rangle$$

where $\widehat{P}_n^{\lambda_o} \equiv |\phi_n^{\lambda_o}\rangle\langle\phi_n^{\lambda_o}|$.

More realistically, the probability would be

$$f_{\phi}^{\lambda_o}(g; n) \equiv \int_{-\pi}^{\pi} g(\lambda)\langle\phi \mid \widehat{P}_n^{\lambda}\phi\rangle d\lambda \tag{2.1}$$

assuming RHS (2.1) is defined. To see that RHS (2.1) is indeed defined we note the following:

$$\langle\phi \mid \widehat{P}_n^{\lambda}\phi\rangle = \frac{1}{L}\left|\int_J e^{-i(2\pi n+\lambda)x/L}\phi(x)dx\right|^2,$$

[1] This operator is often identified with the momentum observable for a particle constrained to move on a circle of circumference L, see for example [29]. However, operators $\widehat{P}^{\lambda}(J)$ for $\lambda \neq 0$ are not appropriate as candidate momentum observables for such a system and the discussion here is relevant only to an interval of the real line. See appendix G for more discussion on this point.

which may be recast in the form

$$\langle \phi \mid \widehat{P}_n^{\lambda} \phi \rangle = \frac{2\pi}{L} \left| \left(\mathcal{F}\overline{\phi} \right) (\lambda / L) \right|^2$$

where

$$\overline{\phi}(x) = \begin{cases} e^{-i2\pi n \frac{x}{L}} \phi(x) & \forall x \in J \\ 0 & \forall x \notin J \end{cases}$$

and $\mathcal{F}\overline{\phi}$ is the Fourier transform of $\overline{\phi}$, i.e.

$$\left(\mathcal{F}\overline{\phi} \right) (\lambda / L) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i \frac{\lambda}{L} x} \overline{\phi}(x) dx.$$

Since $\mathcal{F}$ is an isometric mapping of $L^2(\mathbb{R})$ onto $L^2(\mathbb{R})$ [25, p 59] then $\left| \left(\mathcal{F}\overline{\phi} \right) (\lambda / L) \right|^2$ is integrable on $\mathbb{R}$. It follows that $g(\lambda) \langle \phi \mid \widehat{P}_n^{\lambda} \phi \rangle$ is an integrable function of λ on $(-\pi, \pi]$.

We also have

$$\begin{aligned} \sum_n f_{\phi}^{\lambda_o}(g; n) &= \sum_n \int_{-\pi}^{\pi} g(\lambda) \langle \phi \mid \widehat{P}_n^{\lambda} \phi \rangle d\lambda \\ &= \int_{-\pi}^{\pi} g(\lambda) \sum_n \langle \phi \mid \widehat{P}_n^{\lambda} \phi \rangle d\lambda = \int_{-\pi}^{\pi} g(\lambda) d\lambda = 1, \end{aligned}$$

where we have used proposition 4.4.7 in [63] to enable us to perform the summation inside the integral. So $\{ f_{\phi}^{\lambda_o}(g; n) : n = 0, \pm 1, \pm 2, ... \}$ forms a discrete probability density function. We can formally express $f_{\phi}^{\lambda_o}(g; n)$ thus:

$$f_{\phi}^{\lambda_o}(g; n) = \langle \phi \mid \widehat{F}(\widehat{P}^{\lambda_o}(J), g; n) \phi \rangle$$

where

$$\widehat{F}(\widehat{P}^{\lambda_o}(J), g; n) = \int_{-\pi}^{\pi} d\lambda g(\lambda) \widehat{P}_n^{\lambda}.$$

Now the set

$$\left\{ \widehat{F}(\widehat{P}^{\lambda_o}(J), g; n) : n = 0, \pm 1, \pm 2, ... \right\}$$

constitutes a formal discrete GRI, and it is this object which represents the adapted observable. Of course, it is only the probabilities $f_{\phi}^{\lambda_o}(g; n)$ as given by (2.1) which have any direct physical meaning. We shall now determine the mean and variance of this adapted observable and in doing so demonstrate that the family

$$\left\{ F_{\phi}^{\lambda_o}(g; n) : \phi \in \mathcal{D}(\widehat{P}_o(J)) \right\},$$

where $F_\phi^{\lambda_o}(g;n)$ is the discrete PDF defined by

$$F_\phi^{\lambda_o}(g;n) = \sum_{m=-\infty}^{n} f_\phi^{\lambda_o}(g;m),$$

is not a maximal family of PDFs.

The mean is given by

$$\mathcal{E}(\widehat{P}_o(J), g; \phi) = \sum_n P_n^{\lambda_o} f_\phi^{\lambda_o}(g;n).$$

Now

$$\begin{aligned}
\sum_n P_n^{\lambda_o} f_\phi^{\lambda_o}(g;n) &= \sum_n P_n^{\lambda_o} \int_{-\pi}^{\pi} g(\lambda)\langle \phi \mid \widehat{P}_n^\lambda \phi\rangle d\lambda \\
&= \sum_n \int_{-\pi}^{\pi} P_n^\lambda g(\lambda)\langle \phi \mid \widehat{P}_n^\lambda \phi\rangle d\lambda \\
&+ \sum_n \int_{-\pi}^{\pi} (P_n^{\lambda_o} - P_n^\lambda) g(\lambda)\langle \phi \mid \widehat{P}_n^\lambda \phi\rangle d\lambda \\
&= \langle \phi \mid \widehat{P}_o(J)\phi\rangle + \int_{-\pi}^{\pi} \frac{\hbar}{L}(\lambda_o - \lambda) g(\lambda) d\lambda,
\end{aligned} \tag{2.2}$$

where we have used

$$\int_{-\pi}^{\pi} g(\lambda) d\lambda = \sum_n \langle \phi \mid \widehat{P}_n^\lambda \phi\rangle = 1 \tag{2.3}$$

and

$$\sum_n P_n^\lambda \langle \phi \mid \widehat{P}_n^\lambda \phi\rangle = \langle \phi \mid \widehat{P}_o(J)\phi\rangle. \tag{2.4}$$

Since $\lambda_o = 0 = \int_{-\pi}^{\pi} \lambda g(\lambda) d\lambda$ then the second term of RHS (2.2) is zero and we have

$$\mathcal{E}(\widehat{P}_o(J), g; \phi) = \langle \phi \mid \widehat{P}_o(J)\phi\rangle.$$

The variance is given by

$$\begin{aligned}
\mathcal{V}(\widehat{P}_o(J), g; \phi) &= \sum_n (P_n^{\lambda_o})^2 f_\phi^{\lambda_o}(g;n) - \mathcal{E}(P_o(J), g; \phi)^2 \\
&= \sum_n \int_{-\pi}^{\pi} (P_n^\lambda + P_n^{\lambda_o} - P_n^\lambda)^2 g(\lambda)\langle \phi \mid \widehat{P}_n^\lambda \phi\rangle d\lambda - \langle \phi \mid \widehat{P}_o(J)\phi\rangle^2 \\
&= \sum_n \int_{-\pi}^{\pi} \left\{ (P_n^\lambda)^2 - \left(\frac{2\hbar\lambda}{L}\right) P_n^\lambda + \left(\frac{\hbar\lambda}{L}\right)^2 \right\} g(\lambda)\langle \phi \mid \widehat{P}_n^\lambda \phi\rangle d\lambda - \langle \phi \mid \widehat{P}_o(J)\phi\rangle^2 \\
&= \left\|\widehat{P}_o(J)\phi\right\|^2 + \left(\frac{\hbar}{L}\right)^2 \int_{-\pi}^{\pi} \lambda^2 g(\lambda) d\lambda - \langle \phi \mid \widehat{P}_o(J)\phi\rangle^2,
\end{aligned}$$

where we have used (2.3) and (2.4) as well as

$$\int_{-\pi}^{\pi} \lambda g(\lambda) d\lambda = 0 \text{ and } \sum_n (P_n^\lambda)^2 \langle \phi \mid \widehat{P}_n^\lambda \phi \rangle = \left\| \widehat{P}_o(J)\phi \right\|^2 .$$

So

$$\mathcal{V}(\widehat{P}_o(J), g; \phi) = \mathcal{V}(\widehat{P}_o(J); \phi) + \left(\frac{\hbar}{L}\right)^2 \mathcal{V}(g),$$

where

$$\mathcal{V}(\widehat{P}_o(J); \phi) \equiv \left\| \widehat{P}_o(J)\phi \right\|^2 - \langle \phi \mid \widehat{P}_o(J)\phi \rangle^2 .$$

Hence the mean is unchanged but we have an increase in the variance of $(\hbar/L)^2\mathcal{V}(g)$; clearly

$$\left\{ F_\phi^{\lambda_o}(g; n) : \phi \in \mathcal{D}(\widehat{P}_o(J)) \right\}$$

is not a maximal family.

2.2 Unsharpness and Decomposable Maximal Symmetric Operators

In the previous section an observable had to be adapted to take into account the fact that it may not be distinguished from other observables in a closely related family. We now wish to consider the possibility that the Hilbert space itself may not be sharply defined and see how to adapt observables in this case.

We are to consider the system of an otherwise free particle confined to a semi-infinite interval $J_\omega = [\omega, \infty)$. The appropriate Hilbert space for this system is $\mathcal{H}(\omega) = L^2(J_\omega)$.

Suppose there is some uncertainty as to the precise value of ω, i.e. ω is to be treated as a variable; we will assume it can take any value in a finite interval Ω of $\mathbb{R}$. Physically this corresponds to the constraint at ω not being totally rigid. To describe this we shall employ an extended system, the states of which are to be unit vectors in the direct integral Hilbert space

$$\mathcal{H}^\oplus = \int_\Omega^\oplus \mathcal{H}(\omega) d\omega,$$

and these are denoted by

$$\phi^\oplus = \int_\Omega^\oplus \phi(\omega) d\omega, \qquad \phi(\omega) \in \mathcal{H}(\omega).$$

As the uncertainty in ω is assumed to be due only to our ignorance then not every $\phi^\oplus \in \mathcal{H}^\oplus$ is a valid pure state of the extended system. So a general $\phi^\oplus$ is to be regarded as a mixed state. Indeed there are no pure states at all on account of the continuity of the Lebesgue measure, reflecting the fact that we could never fix ω to a particular value with unlimited precision.

This lack of correspondence between unit vectors and pure states has the form of a 'continuous superselection rule', which is a generalised notion of the more familiar discrete type [64]. Consistency demands that a maximal symmetric operator defined in $\mathcal{H}^\oplus$ can represent an observable for the extended system only if it is decomposable, i.e. it is of the form

$$\widehat{A}^{\oplus} = \int_{\Omega}^{\oplus} \widehat{A}(\omega) d\omega,$$

where $\widehat{A}^{\oplus}$ leaves all subspaces $\mathcal{H}_{\Delta}^{\oplus} \equiv \int_{\Delta \subset \Omega}^{\oplus} \mathcal{H}(\omega) d\omega$ invariant.

Example: The momentum operator for a particle on $[\omega, \infty)$ is given by

$$\mathcal{D}\Big(\widehat{P}(\omega)\Big) = \{\phi \in \mathcal{H}(\omega) : \phi \in AC(\omega, \infty), \phi' \in \mathcal{H}(\omega), \phi(\omega) = 0\}$$

and

$$\widehat{P}(\omega)\phi = -i\hbar \frac{d\phi}{dx} \quad \forall \phi \in \mathcal{D}\Big(\widehat{P}(\omega)\Big),$$

where $\widehat{P}(\omega)$ is maximal symmetric with deficiency indices (1,0).

The momentum operator for the extended system is taken to be

$$\widehat{P}^{\oplus} = \int_{\Omega}^{\oplus} \widehat{P}(\omega) d\omega,$$

which is defined on

$$\mathcal{D}(\widehat{P}^{\oplus}) = \left\{ \phi^{\oplus} \in \mathcal{H}^{\oplus} : \phi(\omega) \in \mathcal{D}\Big(\widehat{P}(\omega)\Big), \int_{\Omega} \left\| \widehat{P}(\omega)\phi(\omega) \right\|_{\omega}^{2} d\omega < \infty \right\}.$$

In the absence of a relevant theorem, we can only surmise that $\widehat{P}^{\oplus}$ is maximal symmetric.[2] In particular, we should stress that $\widehat{P}^{\oplus}$ is not an approximate observable. All the uncertainty associated with ω is built into the state of the extended system.

[2]To add credibility to this conjecture, we give, in appendix H, a generalisation of a result due to Reed and Simon [65, pp 283–284] concerning the self-adjointness of a particular class of direct integral operator.

2.3 Measuring Devices of Limited Range

Any realistic measuring device (MD) is sensitive to only a finite range of observable values. In this section we shall see how to adapt (ideal) observables so that they respect this limitation.

Orthodox Observables

Let $\widehat{A}$ be a not necessarily bounded self-adjoint operator defined in a Hilbert space $\mathcal{H}$ and suppose the MD used to measure $\widehat{A}$ has a finite range $\Lambda = (\lambda_1, \lambda_2]$. Generally, the (maximal) family of PDFs generated by the spectral function of $\widehat{A}$ will not yield the correct description for the measurement of $\widehat{A}$ made with such a device. For a start, the probability of the MD returning a value which lies outside Λ should be zero, but the PDF generated by $\widehat{E}(\widehat{A};\lambda)$ generally contradicts this. The correct probability of obtaining a result in Δ is given by

$$F(\widehat{A}, \Lambda, \phi; \Delta) \equiv \langle \phi \mid \widehat{E}(\widehat{A}; \Delta \cap \Lambda)\phi \rangle,$$

where $F(\widehat{A}, \Lambda, \phi; \Delta)$ is a non-normalised probability measure which agrees with the ideal one if and only if $\Delta \subseteq \Lambda$ and is notably zero if $\Delta \cap \Lambda = \emptyset$. The corresponding non-normalised PDF is

$$F(\widehat{A}, \Lambda, \phi; \lambda) = \langle \phi \mid \widehat{E}(\widehat{A}, \Lambda; \lambda)\phi \rangle$$

where $\widehat{E}(\widehat{A}, \Lambda; \lambda)$ is a non-normalised ORI defined by

$$\widehat{E}(\widehat{A}, \Lambda; \lambda) = \begin{cases} \widehat{E}(\widehat{A}; \lambda_1) & \lambda \leq \lambda_1 \\ \widehat{E}(\widehat{A}; \lambda) & \lambda_1 < \lambda \leq \lambda_2 \\ \widehat{E}(\widehat{A}; \lambda_2) & \lambda > \lambda_2. \end{cases}$$

Let us introduce the operator $\widehat{A}_\Lambda$ defined by

$$\widehat{A}_\Lambda = \int_\Lambda \lambda d_\lambda \widehat{E}(\widehat{A}; \lambda)$$

where $\widehat{A}_\Lambda$ is bounded, self-adjoint and possesses a unique (orthogonal) spectral function $\widehat{E}(\widehat{A}_\Lambda; \lambda)$ defined by

$$\widehat{E}(\widehat{A}_\Lambda; \lambda) = \begin{cases} \widehat{0} & \lambda \leq \lambda_1 \\ \widehat{E}(\widehat{A}; \lambda) & \lambda_1 < \lambda \leq \lambda_2 \\ \widehat{I} & \lambda > \lambda_2. \end{cases}$$

Though $\widehat{A}_\Lambda$ would appear to be a natural choice for the adapted observable, it is obviously not the correct one, since $\widehat{E}(\widehat{A}_\Lambda; \lambda)$ does not coincide with $\widehat{E}(\widehat{A}, \Lambda; \lambda)$. Note however that provided Δ lies in one of the intervals $(-\infty, \lambda_1]$, Λ or (λ_2, ∞) then we may use either of the measures $\widehat{E}(\widehat{A}, \Lambda; \Delta)$ or $\widehat{E}(\widehat{A}_\Lambda; \Delta)$ as they are equivalent. For any other Δ though we must use $\widehat{E}(\widehat{A}, \Lambda; \Delta)$. For example, suppose we wish to measure the momentum $\widehat{P}$ with such a device, here $\mathcal{H} = L^2(\mathbb{R})$. If the state ϕ satisfies $\widehat{E}(\widehat{X}; \Delta')\phi = \phi$ where Δ' is a finite interval of $\mathbb{R}$ then, as is well known, $\widehat{E}(\widehat{P}; \Delta'')\phi = \phi$ is satisfied only if $\Delta'' = \mathbb{R}$. For such a state the probability of obtaining any measured value of momentum should be strictly less than one if the MD is sensitive to only a finite range of momenta. Clearly though $\langle \phi \mid \widehat{E}(\widehat{P}_\Lambda; \mathbb{R})\phi \rangle = 1$ for all ϕ in $\mathcal{H}$ and so generally $\widehat{E}(\widehat{A}_\Lambda; \lambda)$ is not the appropriate choice for the adapted observable. A proper description is given only in terms of the non-normalised ORI $\widehat{E}(\widehat{A}, \Lambda; \lambda)$. We conclude that the relevant adapted observable is $\widehat{E}(\widehat{A}, \Lambda; \lambda)$ though $\widehat{A}_\Lambda$ may be used with caution.

Generalised Observables

Now suppose $\widehat{A}$ is maximal symmetric but not necessarily self-adjoint. The adapted observable in this case is the non-normalised GRI

$$\widehat{F}(\widehat{A}, \Lambda; \lambda) = \begin{cases} \widehat{F}(\widehat{A}; \lambda_1) & \lambda \leq \lambda_1 \\ \widehat{F}(\widehat{A}; \lambda) & \lambda_1 < \lambda \leq \lambda_2 \\ \widehat{F}(\widehat{A}; \lambda_2) & \lambda > \lambda_2 \end{cases}$$

where $\widehat{F}(\widehat{A}; \lambda)$ is the generalised spectral function of $\widehat{A}$. Next we shall seek an operator $\widehat{A}_\Lambda$ analogous to that for the self-adjoint case. Recall that for $\widehat{A}$ self-adjoint, Λ bounded and ϕ an arbitrary element of $\mathcal{H}$, we have

$$\widehat{E}(\widehat{A};\Lambda)\phi \in \mathcal{D}(\widehat{A}), \tag{2.5}$$

$$\widehat{A}_\Lambda\phi = \widehat{A}\widehat{E}(\widehat{A};\Lambda)\phi \tag{2.6}$$

and if $\phi \in \mathcal{D}(\widehat{A})$ then

$$\widehat{A}_\Lambda\phi = \widehat{E}(\widehat{A};\Lambda)\widehat{A}\phi. \tag{2.7}$$

It is not at all obvious that (2.5), (2.6) and (2.7) can be extended to apply in the general case where $\widehat{A}$ need not be self-adjoint. It turns out that [11, p 133]

$$\widehat{F}(\widehat{A};\Lambda)\phi \in \mathcal{D}(\widehat{A}^\dagger) \quad \forall\phi \in \mathcal{H},$$

and, furthermore, we have

$$\langle\psi \mid \widehat{A}^\dagger\widehat{F}(\widehat{A};\Lambda)\phi\rangle = \int_\Lambda \lambda d_\lambda\langle\psi \mid \widehat{F}(\widehat{A};\lambda)\phi\rangle \quad \forall\psi,\phi \in \mathcal{H}.$$

Now since $\widehat{A}_\Lambda \equiv \widehat{A}^\dagger\widehat{F}(\widehat{A};\Lambda)$ is defined *on* $\mathcal{H}$, it is bounded, and as $\langle\phi \mid \widehat{A}_\Lambda\phi\rangle$ is real for all ϕ in $\mathcal{H}$ then $\widehat{A}_\Lambda$ is symmetric [58, p 72]. Hence $\widehat{A}_\Lambda$ is self-adjoint.

Also if we define $\widehat{A}^o_\Lambda$ on $\mathcal{D}(\widehat{A})$ by

$$\widehat{A}^o_\Lambda = \widehat{F}(\widehat{A};\Lambda)\widehat{A},$$

where $\widehat{A}^o_\Lambda$ is symmetric in $\mathcal{H}$, then [61, pp 300–301]

$$(\widehat{A}^o_\Lambda)^\dagger = \widehat{A}^\dagger\widehat{F}(\widehat{A};\Lambda) = \widehat{A}_\Lambda,$$

i.e. $\widehat{A}^o_\Lambda$ is essentially self-adjoint with unique self-adjoint extension $\widehat{A}_\Lambda$, this being the closure of $\widehat{A}^o_\Lambda$. So $\widehat{A}_\Lambda = \widehat{F}(\widehat{A};\Lambda)\widehat{A}$ on $\mathcal{D}(\widehat{A})$ and this completes the generalisation of (2.5) to (2.7). Now unless $\widehat{A}$ is self-adjoint then $\widehat{A}_\Lambda$ is of little use. Clearly, as $\widehat{A}_\Lambda$ is self-adjoint, $\widehat{E}(\widehat{A}_\Lambda;\lambda)$ is an ORI. So even if $\Delta \in \Lambda$ we generally do not have

$$\widehat{F}(\widehat{A},\Lambda;\Delta) = \widehat{E}(\widehat{A}_\Lambda;\Delta)$$

since the LHS need not be projector valued.

As a sideline we note that for $\phi \in \mathcal{D}(\widehat{A})$ and for a partition $\{\Lambda_i\}$ of $\mathbb{R}$, we have

$$\begin{aligned}\langle \phi \mid \widehat{A}\phi \rangle &= \sum_i \langle \widehat{F}(\widehat{A};\Lambda_i)\phi \mid \widehat{A}\phi \rangle \\ &= \sum_i \langle \widehat{A}^\dagger \widehat{F}(\widehat{A};\Lambda_i)\phi \mid \phi \rangle \\ &= \sum_i \langle \phi \mid \widehat{A}_{\Lambda_i}\phi \rangle .\end{aligned}$$

We can thus obtain the expectation value of $\widehat{A}$ by measuring observables which are represented by self-adjoint operators. Here we are presented with the possibility that a general maximal symmetric operator, which is associated with a POV measure, may be approximated by a self-adjoint operator, which is associated with a PV measure. Indeed, as remarked in chapter 1, Wan and McLean [26] have recently shown that the mean value of an arbitrary orthodox observable, i.e. a self-adjoint operator, can be obtained to an arbitrary degree of accuracy by local orthodox position measurements. So, in principle, measurement of generalised observables may be approximated by local position measurements.

In the next section we consider a more drastic customisation of ideal observables which also results in a description of measurement in terms of non-normalised POV measures.

2.4 Local Observables

Motivated by the fact that all realistic measuring devices (MDs) are of finite spatial extent, Wan and Jackson [66], following Haag and Kastler's introduction of local observables in quantum field theory [67], proposed a scheme whereby this limitation manifests itself in the observables measurable with such a device. Given an orthodox observable which can be represented by a bounded self-adjoint operator, this is *adapted* to an MD of a particular size by a *localisation procedure.*

Definition 11 *Let $\widehat{A}$ be a bounded self-adjoint operator defined on $L^2(\mathbb{R})$ and let J be a finite interval of $\mathbb{R}$. If*

$$\widehat{A} = \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J)$$

then $\widehat{A}$ is called a bounded local observable in J.

The localisation of $\widehat{A}$ to J is defined by

$$\widehat{A}_J = \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J) \tag{2.8}$$

where $\widehat{A}_J$ is clearly a uniquely defined bounded local observable in J.

So, in Wan and Jackson's scheme, all observables represented by bounded self-adjoint operators defined on $L^2(\mathbb{R})$ that are measurable with a device of size J are assumed to be local observables in J.

As remarked elsewhere [35] the localisation process cannot be directly extended to unbounded self-adjoint operators for two reasons: Firstly the range of $\widehat{E}(\widehat{X};J)$ may not be a dense subset of the domain of $\widehat{A}$ and secondly even if $\widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J)$ is densely defined it may not be self-adjoint and may not even possess self-adjoint extensions. To circumvent this it was proposed in [66] that the localisation process be applied to the spectral measures of unbounded self-adjoint operators. However this gives rise to further problems such as a localised projector will not necessarily be a projector itself.

Wan and coworkers have since developed other more elaborate strategies for localising unbounded self-adjoint operators directly. However, in view of our generalised notion of observable which need not be associated with a self-adjoint operator or with a PV measure, we shall reconsider the scheme of Wan and Jackson and promote localised observables as examples of adapted observables. We shall also consider a weaker notion of local observable than that in [66] which ties in with Wan and Sumner's concept of local values [69, 70].

2.4.1 Local POV Measures

We can apply (2.8) to each projector in the range of the spectral measure $\widehat{E}(\widehat{A};\cdot)$ of a self-adjoint operator $\widehat{A}$ defined in $L^2(\mathbb{R})$. This yields the non-normalised POV measure $\widehat{E}_J(\widehat{A};\cdot)$ defined on the Borel sets Δ of $\mathbb{R}$ by

$$\widehat{E}_J(\widehat{A};\Delta) = \widehat{E}(\widehat{X};J)\widehat{E}(\widehat{A};\Delta)\widehat{E}(\widehat{X};J).$$

We then interpret $\widehat{E}_J(\widehat{A};\cdot)$ as describing the measurement of observable $\widehat{A}$ with an MD of finite spatial extent J. In other words $\widehat{E}_J(\widehat{A};\cdot)$ is an adapted observable which respects the finite size of the MD as characterised in [66]. So the probability of obtaining a measured value in Δ when the state of the system is ϕ is given by

$$\wp_J(\widehat{A},\phi;\Delta) = \langle \phi \mid \widehat{E}_J(\widehat{A};\Delta)\phi\rangle.$$

With this interpretation, the fact that $\widehat{E}_J(\widehat{A};\Delta)$ is not normalised, i.e. $\widehat{E}_J(\widehat{A};\mathbb{R}) < \widehat{I}$, is not a problem since $\wp_J(\widehat{A},\phi;\mathbb{R}) = \langle \phi \mid \widehat{E}(\widehat{X};J)\phi\rangle$ is just the probability that upon measurement, the system in state ϕ is found to lie in J.[3]

We wish now to attempt to localise an unbounded observable in a similar way to how we would for a bounded observable. Specifically, we wish to consider the possibility of localising the momentum operator $\widehat{P}$ to an interval $J = [j_1, j_2]$ where $-\infty < j_1 < j_2 < \infty$. Recall that $\widehat{P}$ is defined on

$$\mathcal{D}(\widehat{P}) = \left\{\phi \in L^2(\mathbb{R}) : \phi \in AC(\mathbb{R}), \phi' \in L^2(\mathbb{R})\right\}$$

by

$$\widehat{P}\phi = -i\hbar\frac{d\phi}{dx}.$$

[3]Prugovečki also advocates, though for different reasons, the use of non-normalised POV measures for the representation of observables [28, p 65].

If we attempt to localise $\widehat{P}$ to J we immediately run into domain problems since if $\phi \in AC(\mathbb{R})$ then $\widehat{E}(\widehat{X}; J)\phi \in AC(\mathbb{R})$ if and only if $\phi(j_1) = \phi(j_2) = 0$. So we tentatively define $\widehat{P}_J$ by

$$\mathcal{D}(\widehat{P}_J) = \left\{\phi \in \mathcal{D}(\widehat{P}) : \phi(j_1) = \phi(j_2) = 0\right\}$$

and

$$\widehat{P}_J\phi = \widehat{E}(\widehat{X}; J)\widehat{P}\widehat{E}(\widehat{X}; J)\phi \qquad \forall\phi \in \mathcal{D}(\widehat{P}_J).$$

Introduce the operator $\widetilde{P}_J$ defined by

$$\mathcal{D}(\widetilde{P}_J) = \mathcal{D}(\widehat{P}_J)$$

and

$$\widetilde{P}_J\phi = \widehat{P}\phi \qquad \forall\phi \in \mathcal{D}(\widetilde{P}_J).$$

One can easily show (follow the proof in [21, pp 106–108]) that $\widetilde{P}_J^\dagger = \widehat{P}$, i.e. $\widetilde{P}_J$ is essentially self-adjoint with unique self-adjoint extension $\widehat{P}$. Now since

$$\mathcal{D}(\widehat{P}_J) = \left\{\phi \in \mathcal{D}(\widetilde{P}_J) : \widetilde{P}_J\phi \in \mathcal{D}\Big(\widehat{E}(\widehat{X}; J)\Big)\right\}$$

and

$$\widehat{P}_J\phi = \widehat{E}(\widehat{X}; J)\widetilde{P}_J\phi \qquad \forall\phi \in \mathcal{D}(\widehat{P}_J),$$

then it follows [61, pp 298–301] that

$$\widehat{P}_J^\dagger = \widetilde{P}_J^\dagger\widehat{E}(\widehat{X}; J)^\dagger = \widehat{P}\widehat{E}(\widehat{X}; J)$$

with domain

$$\mathcal{D}(\widehat{P}_J^\dagger) = \left\{\phi \in \mathcal{D}\Big(\widehat{E}(\widehat{X}; J)\Big) : \widehat{E}(\widehat{X}; J)\phi \in \mathcal{D}(\widehat{P})\right\}$$
$$= \left\{\phi \in L^2(\mathbb{R}) : \phi \in AC(J), \phi' \in L^2(\mathbb{R}), \phi(j_1) = \phi(j_2) = 0\right\}.$$

So we have,

$$\mathcal{D}(\widehat{P}_J) = \mathcal{D}(\widehat{P}_J^\dagger) \cap AC(J^c) \subset \mathcal{D}(\widehat{P}_J^\dagger)$$

and

$$\widehat{P}_J^\dagger\phi = \widehat{P}_J\phi \qquad \forall\phi \in \mathcal{D}(\widehat{P}_J).$$

Hence $\widehat{P}_J^\dagger \supset \widehat{P}_J$ and $\widehat{P}_J$ is a non-maximal symmetric operator. Clearly $\widehat{E}_J(\widehat{P};\lambda)$ cannot be a (generalised) spectral function of $\widehat{P}_J$ since $\lim_{\lambda\to\infty}\widehat{E}_J(\widehat{P};\lambda) \neq \widehat{I}$. However, we do have, for arbitrary $\phi \in \mathcal{D}(\widehat{P}_J)$ and $\psi \in L^2(\mathbb{R})$, the following

$$\int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{E}_J(\widehat{P};\lambda)\phi\rangle < \infty,$$

$$\langle \psi \mid \widehat{P}_J\phi\rangle = \int_{-\infty}^{\infty} \lambda d_\lambda \langle \psi \mid \widehat{E}_J(\widehat{P};\lambda)\phi\rangle$$

and

$$\left\|\widehat{P}_J\phi\right\|^2 = \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{E}_J(\widehat{P};\lambda)\phi\rangle.$$

Note that although $\widehat{P}_J$ possesses maximal symmetric extensions which can serve as observables, it is the non-normalised POV measure $\widehat{E}_J(\widehat{P};\cdot)$ which is the appropriate adapted observable.

Those localised PV measures which are themselves projector valued are revealed by the following [17]

Proposition: *If $\widehat{P}_1$ and $\widehat{P}_2$ are projectors defined on the same Hilbert space $\mathcal{H}$ then $\widehat{P}_1\widehat{P}_2\widehat{P}_1$ is a projector on $\mathcal{H}$ if and only if $\widehat{P}_1$ and $\widehat{P}_2$ commute.*

So, for example, the non-normalised POV measure $\widehat{E}_J(\widehat{P};\cdot)$ is not projector valued.

2.4.2 Weakly Local POV Measures

Definition 12 *The local decomposition of a bounded operator $\widehat{A}$ defined on $L^2(\mathbb{R})$ with respect to a finite interval J is defined to be*

$$\widehat{A} = \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J) + \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J^c)$$

$$+\, \widehat{E}(\widehat{X};J^c)\widehat{A}\widehat{E}(\widehat{X};J) + \widehat{E}(\widehat{X};J^c)\widehat{A}\widehat{E}(\widehat{X};J^c), \qquad J^c = \mathbb{R} - J. \tag{2.9}$$

Definition 13 *If $\widehat{A}$ is a bounded operator defined on $L^2(\mathbb{R})$ such that its local decomposition with respect to a finite interval J consists of the first three terms only, i.e. $\widehat{E}(\widehat{X};J^c)\widehat{A}\widehat{E}(\widehat{X};J^c) = \widehat{0}$, then $\widehat{A}$ is called weakly local in J.*

Clearly all local operators are weakly local but the converse is not true. The crucial difference between local and weakly local operators is that the latter allow correlations between J and J^c in the sense that for ϕ_J of support in J only and ψ_{J^c} of support in J^c only, $\langle \phi_J \mid \widehat{A}\psi_{J^c}\rangle$ and $\langle \psi_{J^c} \mid \widehat{A}\phi_J\rangle$ need not vanish for $\widehat{A}$ weakly local in J whereas they do vanish for $\widehat{A}$ local in J.

We can introduce a weak localisation procedure analogous to the localisation procedure of definition 11.

Definition 14 *The weak localisation of a bounded operator $\widehat{A}$ defined on $L^2(\mathbb{R})$ to a finite interval J is defined by*

$$\widehat{A}_{W_J} = \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J) + \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J^c) + \widehat{E}(\widehat{X};J^c)\widehat{A}\widehat{E}(\widehat{X};J),$$

or, equivalently,

$$\widehat{A}_{W_J} = \widehat{A} - \widehat{E}(\widehat{X};J^c)\widehat{A}\widehat{E}(\widehat{X};J^c).$$

If a bounded operator $\widehat{A}$, defined on $L^2(\mathbb{R}) \equiv \mathcal{H}$, is localised to J to yield $\widehat{A}_J$ and weakly localised to J to yield $\widehat{A}_{W_J}$ then we have

$$\langle \phi_J \mid \widehat{A}_J\phi_J\rangle = \langle \phi_J \mid \widehat{A}_{W_J}\phi_J\rangle = \langle \phi_J \mid \widehat{A}\phi_J\rangle$$

and

$$\begin{aligned}\langle \psi_{J^c} \mid \widehat{A}_J\psi_{J^c}\rangle = \langle \psi_{J^c} \mid \widehat{A}_{W_J}\psi_{J^c}\rangle &= 0 \\ &\neq \langle \psi_{J^c} \mid \widehat{A}\psi_{J^c}\rangle \text{ generally,}\end{aligned}$$

where ϕ_J and ψ_{J^c} are as above.

If $J' \subset J$ then

$$\widehat{A}_{J'} = (\widehat{A}_J)_{J'}$$

and

$$\widehat{A}_{W_{J'}} = (\widehat{A}_{W_J})_{W_{J'}}.$$

In other words if we localise (weakly localise) $\widehat{A}$ to an interval J and then to an interval J' contained in J, this is equivalent to localising (weakly localising) $\widehat{A}$ directly to J'. This 'isotony' property is clearly an important one, especially for the interpretation of local observables. It ensures consistency between measurements made with MDs of size J and $J' \subset J$ for states with support contained in J'.

Note that for an arbitrary $\phi \in \mathcal{H}$, although $\left(\widehat{A}_{W_J}\phi\right)(x)$ for $x \in J$ depends on the value of $\phi(x)$ for $x \in J^c$, this is clearly not so for $\left(\widehat{A}_J\phi\right)(x)$ in view of the fact that $\widehat{A}_J$ and $\widehat{E}(\widehat{X}; J)$ commute. In particular we have for general $\phi \in \mathcal{H}$,

$$\left(\widehat{A}_{W_J}\phi\right)(x) = \left(\widehat{A}\phi\right)(x) \neq \left(\widehat{A}_J\phi\right)(x) \text{ for } x \in J.$$

We will see shortly that attempting to introduce weakly local POV measures as adapted observables and thus extend the notion of local observable is not straightforward. Indeed we shall show that all (non-normalised or otherwise) POV measures which are weakly local are in fact local.

Though the introduction of weakly local operators may be justifiable on grounds of generality, further study would be of only mathematical interest were it not for the existence of a class of observable represented by weakly local, but not necessarily local, operators. Such observables arise naturally if we want to attach physical meaning to the local values of Wan and Sumner, the theory of which we outline next.

2.4.3 Local Values and Semilocal Operators

In an attempt to overcome some of the difficulties associated with Bohm theory, Wan and Sumner [69] introduced the concept of 'spatial distribution of observable values'. This led to the notion of 'local values' [70]. The idea is as follows.

Suppose we partition the real line $\boldsymbol{R}$ into a union of disjoint intervals $\{J_i\}$ i.e. $\boldsymbol{R} = \cup_i J_i$ and $J_i \cap J_j = \emptyset$, $i \neq j$, where all the J_i are assumed to be of finite length. If $\widehat{A}$ is a bounded self-adjoint operator defined on $\mathcal{H} = L^2(\boldsymbol{R})$ then we have for every $\phi \in \mathcal{H}$ the following decomposition,

$$\langle \phi \mid \widehat{A}\phi \rangle = \sum_i \langle \phi \mid \widehat{A}_{J_i}\phi \rangle$$

where

$$\widehat{A}_{J_i} = \frac{1}{2}\left\{\widehat{A}\widehat{E}(\widehat{X};J_i) + \widehat{E}(\widehat{X};J_i)\widehat{A}\right\}.$$

For a given i the value $\langle\phi \mid \widehat{A}_{J_i}\phi\rangle$ is called the local value of $\widehat{A}$ in J_i and, on account of $\widehat{A}_{J_i}$ being self-adjoint, this is the expectation value of the orthodox quantum observable represented by $\widehat{A}_{J_i}$. We shall call operators of the form

$$\widehat{A}_{S_J} = \frac{1}{2}\left\{\widehat{E}(\widehat{X};J)\widehat{A} + \widehat{A}\widehat{E}(\widehat{X};J)\right\}$$

semilocal operators. Clearly if $\widehat{A}_{S_J}$ is semilocal then

$$\widehat{E}(\widehat{X};J^c)\widehat{A}_{S_J}\widehat{E}(\widehat{X};J^c) = \widehat{0}$$

and

$$\widehat{E}(\widehat{X};J)\widehat{A}_{S_J}\widehat{E}(\widehat{X};J) = \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J) \neq \widehat{A}_{S_J} \text{ generally.}$$

So a semilocal operator is an example of a weakly local operator which need not be local. For $\widehat{A}$ self-adjoint, $\widehat{A}_{S_J}$ is then an example of a weakly local observable in J and this gives physical meaning to the local value $\langle\phi \mid \widehat{A}_{S_J}\phi\rangle$. So the expectation value of an arbitrary orthodox observable which may be represented by a bounded self-adjoint operator can be obtained from expectation values of semilocal observables.

There are two outstanding difficulties with this scheme. The first concerns the same difficulty we encountered with local operators in extending these ideas to cater for unbounded operators, in that $\widehat{A}_{S_J}$ for unbounded self-adjoint $\widehat{A}$ is generally only symmetric and may not possess a self-adjoint extension. Allowing maximal symmetric operators to represent observables overcomes some of these problems. The second difficulty has to do with the interpretation of the local values themselves. For example, if we take $\widehat{A} = \widehat{E}(\widehat{P};\Delta)$ where $\widehat{E}(\widehat{P};\cdot)$ is the spectral measure of $\widehat{P}$ then, as we shall see, the local value $\langle\phi \mid \widehat{E}_{S_J}(\widehat{P};\Delta)\phi\rangle$ where $\widehat{E}_{S_J}(\widehat{P};\Delta) = (1/2)\{\widehat{E}(\widehat{X};J)\widehat{E}(\widehat{P};\Delta) + \widehat{E}(\widehat{P};\Delta)\widehat{E}(\widehat{X};J)\}$ may be negative. So although the 'global value' $\langle\phi \mid \widehat{E}(\widehat{P};\Delta)\phi\rangle$ may be interpreted as a probability, the local values generally cannot. These local 'negative probabilities' would still be measurable since they are expectation values of self-adjoint operators and can be regarded as local contributions to the overall (global) probability even though individually they cannot represent probabilities in the usual sense; cf. [71].

Theorem 12 *Every positive weakly local operator defined on $L^2(\mathbb{R})$ is local.*

Proof: Let $\widehat{A}$ be a bounded operator defined on $\mathcal{H} = L^2(\mathbb{R})$ which is weakly local in an interval J of $\mathbb{R}$, i.e.

$$\widehat{A} = \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J) + \widehat{E}(\widehat{X};J^c)\widehat{A}\widehat{E}(\widehat{X};J) + \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J^c).$$

If $\widehat{A}$ is positive, i.e.

$$\langle \phi \mid \widehat{A}\phi \rangle \geq 0 \qquad \forall \phi \in \mathcal{H}$$

then the generalised Schwartz inequality [61, p 262] is satisfied, that is:

$$|\langle \psi \mid \widehat{A}\phi \rangle|^2 \leq \langle \psi \mid \widehat{A}\psi \rangle \langle \phi \mid \widehat{A}\phi \rangle \qquad \forall \psi, \phi \in \mathcal{H}. \tag{2.10}$$

Suppose $\phi = \widehat{E}(\widehat{X};J^c)\eta$ where η is an arbitrary element of $\mathcal{H}$, then we have

$$\langle \phi \mid \widehat{A}\phi \rangle = 0$$

and it follows from (2.10) that

$$|\langle \psi \mid \widehat{A}\phi \rangle|^2 \leq 0,$$

i.e.

$$\langle \psi \mid \widehat{A}\widehat{E}(\widehat{X};J^c)\eta \rangle = 0 \qquad \forall \psi, \eta \in \mathcal{H}.$$

So now we have,

$$\widehat{A}\widehat{E}(\widehat{X};J^c) = \widehat{0}$$

and

$$\widehat{E}(\widehat{X};J^c)\widehat{A} = \left(\widehat{A}\widehat{E}(\widehat{X};J^c)\right)^\dagger = \widehat{0},$$

where we have used the fact that $\widehat{A}$ is self-adjoint on account of it being a positive operator defined on $\mathcal{H}$. Hence

$$\widehat{A} = \widehat{E}(\widehat{X};J)\widehat{A}\widehat{E}(\widehat{X};J),$$

i.e. $\widehat{A}$ is local in J.

To see that for arbitrary J and arbitrary Δ, the local value $\langle\phi \mid \widehat{E}_{S_J}(\widehat{P};\Delta)\phi\rangle$ is negative for some $\phi \in L^2(\mathbb{R})$, we note that

$$\left[\widehat{E}_{S_J}(\widehat{P};\Delta), \widehat{E}(\widehat{X};J)\right] = \frac{1}{2}\left[\widehat{E}(\widehat{P};\Delta), \widehat{E}(\widehat{X};J)\right],$$

which, as is well known, does not coincide with the zero operator $\widehat{0}$. Clearly, an operator which is local in J commutes with $\widehat{E}(\widehat{X};J)$, so $\widehat{E}_{S_J}(\widehat{P};\Delta)$, though weakly local in J, is not local in J. Hence, by theorem 12, $\langle\phi \mid \widehat{E}_{S_J}(\widehat{P};\Delta)\phi\rangle$ is not positive for all ϕ in $L^2(\mathbb{R})$.

This result is not an unexpected one in view of the many no-go theorems preventing a true phase-space formulation of quantum mechanics [2, 45, 72, 73]. For example, introduce the operator-valued set function $\widehat{B}(\Delta \times J)$ defined on the phase space $\Gamma = \mathbb{R} \times \mathbb{R}$ by

$$\widehat{B}(\Delta \times J) = \widehat{E}_{S_J}(\widehat{P};\Delta).$$

This can be extended to a measure on Γ in the usual manner, the marginals of which are given by

$$\widehat{B}(\Delta \times \mathbb{R}) = \widehat{E}(\widehat{P};\Delta)$$

$$\widehat{B}(\mathbb{R} \times J) = \widehat{E}(\widehat{X};J).$$

Now since $\widehat{B}(\Delta \times \mathbb{R})$ and $\widehat{B}(\mathbb{R} \times J)$ are non-commuting projectors then, by theorem 2.1 in [2, p 39], $\widehat{E}_{S_J}(\widehat{P};\Delta)$ cannot be a positive operator for all $\Delta \times J$.

2.4.4 Field-Operators

We are to consider here the apparent locality implicit in the field-operator formulation of orthodox quantum mechanics [74]. The field-operators $\widetilde{\psi}^\dagger(x)$ and $\widetilde{\psi}(x)$ are respectively interpreted as effecting the creation and annihilation of a particle at the point $x \in \mathbb{R}$ [75, pp 133–134]. If $\{u_k\}$ is an orthonormal basis for the single-particle Hilbert space $\mathcal{H}^{(1)} \equiv L^2(\mathbb{R})$, then $\widetilde{\psi}^\dagger(x)$ and $\widetilde{\psi}(x)$ are defined on the corresponding Fock space $\mathcal{H}^F$ by

$$\widetilde{\psi}^\dagger(x) = \sum_k u_k^*(x)\widetilde{a}_k^\dagger$$

$$\widetilde{\psi}(x) = \sum_k u_k(x)\widetilde{a}_k,$$

where $\widetilde{a}_k^\dagger$ and $\widetilde{a}_k$ are the creation and annihilation operators for a state $|1_k\rangle$ in $\mathcal{H}^F$ which corresponds to the element u_k of $\mathcal{H}^{(1)}$. Assuming the relevant particles are bosons then $\widetilde{a}_k^\dagger$ and $\widetilde{a}_k$ satisfy the commutation relations

$$\left[\widetilde{a}_k, \widetilde{a}_l^\dagger\right] = \delta_{kl}\widetilde{I}$$

$$[\widetilde{a}_k, \widetilde{a}_l] = \left[\widetilde{a}_k^\dagger, \widetilde{a}_l^\dagger\right] = \widetilde{0},$$

where $\widetilde{I}$ and $\widetilde{0}$ are the identity and zero operators on $\mathcal{H}^F$. For the field-operators $\widetilde{\psi}^\dagger(x)$ and $\widetilde{\psi}(x)$ we then have

$$\left[\widetilde{\psi}(x), \widetilde{\psi}^\dagger(x')\right] = \delta(x - x')\widetilde{I}$$

$$\left[\widetilde{\psi}(x), \widetilde{\psi}(x')\right] = \left[\widetilde{\psi}^\dagger(x), \widetilde{\psi}^\dagger(x')\right] = \widetilde{0}.$$

The field-operator representation of a self-adjoint operator $\widehat{A}$ defined in $\mathcal{H}^{(1)}$ is given by

$$\widetilde{A} = \int_{-\infty}^{\infty} dx\, \widetilde{\psi}^\dagger(x)\widehat{A}\widetilde{\psi}(x). \tag{2.11}$$

To see the equivalence of the two representations we note the following. Let $|1_p\rangle$ and $|1_q\rangle$ be single-particle states in $\mathcal{H}^F$ corresponding to u_p and u_q in $\mathcal{H}^{(1)}$. We have

$$\widetilde{A}|1_q\rangle = \int_{-\infty}^{\infty} dx\, \widetilde{\psi}^\dagger(x) \sum_k \left(\widehat{A}u_k\right)(x)\widetilde{a}_k|1_q\rangle$$

and since $\widetilde{a}_k|1_q\rangle = \delta_{kq}|0\rangle$, where $|0\rangle$ denotes the vacuum state, then

$$\widetilde{A}|1_q\rangle = \int_{-\infty}^{\infty} dx\, \left(\widehat{A}u_q\right)(x) \sum_k u_k^*(x)|1_k\rangle,$$

so that

$$\begin{aligned}
\langle 1_p|\widetilde{A}|1_q\rangle &= \int_{-\infty}^{\infty} dx\, u_p^*(x)\left(\widehat{A}u_q\right)(x) \\
&= \langle u_p \mid \widehat{A}u_q\rangle.
\end{aligned}$$

In view of the fact that $\widetilde{A}$, as given by (2.11), has the form of an integrated density on $\mathbb{R}$, it is tempting to view $\widetilde{A}_J$ defined by

$$\widetilde{A}_J = \int_J dx\, \widetilde{\psi}^\dagger(x)\widehat{A}\widetilde{\psi}(x),$$

where J is a finite interval of $\mathbb{R}$, as a kind of local observable associated with J. However, $\widetilde{A}_J$ is generally not self-adjoint. This becomes clear when $\widetilde{A}_J$ is expressed in terms of the creation and annihilation operators $\widetilde{a}_k^\dagger$ and $\widetilde{a}_k$. We then have

$$\begin{aligned}\widetilde{A}_J &= \sum_k \sum_l \int_J dx\, u_k^*(x) \left(\widehat{A}u_l\right)(x)\widetilde{a}_k^\dagger \widetilde{a}_l \\ &= \sum_k \sum_l \langle \widehat{E}(\widehat{X}; J)u_k \mid \widehat{A}u_l\rangle \widetilde{a}_k^\dagger \widetilde{a}_l\end{aligned}$$

and

$$\widetilde{A}_J^\dagger = \sum_k \sum_l \langle \widehat{A}u_k \mid \widehat{E}(\widehat{X}; J)u_l\rangle \widetilde{a}_k^\dagger \widetilde{a}_l.$$

Hence

$$\langle 1_p|(\widetilde{A}_J^\dagger - \widetilde{A}_J)|1_q\rangle = \langle u_p \mid (\widehat{A}\widehat{E}(\widehat{X}; J) - \widehat{E}(\widehat{X}; J)\widehat{A})u_q\rangle,$$

which is zero for arbitrary $u_p, u_q \in \mathcal{H}^{(1)}$ if and only if $\widehat{A}$ and $\widehat{E}(\widehat{X}; J)$ commute. This is true in particular if $\widehat{A}$ is local in J in the sense of definition 11. For example, consider the case where $\widehat{A}$ is the identity operator on $\mathcal{H}^{(1)}$. We have

$$\widetilde{A}_J = \int_J dx\, \widetilde{\psi}^\dagger(x)\widetilde{\psi}(x) = \int_{-\infty}^{\infty} dx\, \widetilde{\psi}^\dagger(x)\chi_J(x)\widetilde{\psi}(x),$$

and so $\widetilde{A}_J$ is just the field-operator representation of $\widehat{E}(\widehat{X}; J)$. Now since the particle-number operator $\widetilde{N}$ is given by

$$\widetilde{N} = \int_{-\infty}^{\infty} dx\, \widetilde{\psi}^\dagger(x)\widetilde{\psi}(x),$$

then it is usual to interpret $\widetilde{A}_J$ as the particle-number operator for J [76, p 43]. In other words, the eigenvalues of $\widetilde{A}_J$ are taken to be the possible numbers of particles in J. The validity of this interpretation is borne out by the following illustration [77]:

Using the commutation relations involving $\widetilde{\psi}^\dagger(x)$ and $\widetilde{\psi}(x')$ one arrives at

$$\widetilde{A}_J\widetilde{\psi}(x) = \widetilde{\psi}(x)\widetilde{A}_J - \int_J dx'\, \delta(x - x')\widetilde{\psi}(x')$$

and

$$\widetilde{A}_J\widetilde{\psi}^\dagger(x) = \widetilde{\psi}^\dagger(x)\widetilde{A}_J + \int_J dx'\, \delta(x - x')\widetilde{\psi}^\dagger(x').$$

So that if $|\phi\rangle$ is an eigenstate of $\widetilde{A}_J$ with corresponding eigenvalue n_J then

$$\widetilde{A}_J\widetilde{\psi}(x)|\phi\rangle = \begin{cases} (n_J - 1)\widetilde{\psi}(x)|\phi\rangle & x \in J \\ n_J\widetilde{\psi}(x)|\phi\rangle & x \notin J \end{cases}$$

and

$$\widetilde{A}_J\widetilde{\psi}^\dagger(x)|\phi\rangle = \begin{cases} (n_J + 1)\widetilde{\psi}^\dagger(x)|\phi\rangle & x \in J \\ n_J\widetilde{\psi}^\dagger(x)|\phi\rangle & x \notin J. \end{cases}$$

In the context of non-relativistic quantum field theory, where the field operators $\widetilde{\psi}^\dagger(x)$ and $\widetilde{\psi}(x)$ are obtained by a 'second quantisation' of the free Schrödinger field [78, § 1.7], seemingly local observables emerge quite naturally. Take for instance the field Hamiltonian in one dimension and at time $t = 0$. This is given by [75, p 148]:

$$\mathbf{H} = \int_{-\infty}^{\infty} dx \mathbf{H}(x),$$

where

$$\mathbf{H}(x) = -\frac{\hbar^2}{2m}\widetilde{\psi}^\dagger(x)\frac{d^2}{dx^2}\widetilde{\psi}(x).$$

So $\mathbf{H}$ is just the one-dimensional free particle Hamiltonian $\widehat{H} = -(\hbar^2/2m)d^2/dx^2$ lifted up to the field via eqn (2.11). Now $\widehat{H}$ is formally a local operator and so one can justify the interpretation of $\mathbf{H}(x)$ as a local observable density in that $\int_J dx\mathbf{H}(x)$, where J is an arbitrary finite interval, is formally self-adjoint. A similar interpretation does not however apply to all field observables. For example, consider lifting up to the field the self-adjoint operator $\widehat{E}(\widehat{P};\Delta)$ for finite Δ. As we know, 'chopping off' the integral does not yield a self-adjoint operator even formally on account of the non-commutativity between $\widehat{E}(\widehat{P};\Delta)$ and $\widehat{E}(\widehat{X};J)$ for arbitrary finite J. Generally then, quantum field theory cannot be considered a local theory insofar as physical meaning cannot always be given to the densities which arise as the integrands of the corresponding integrated observables. In particular, lifting up observables from quantum mechanics to quantum field theory does not introduce any extra locality.

Appendix G: Momentum Operators for a Particle on a Circle and a Particle on an Interval

In this appendix we wish to clarify a remark made in section 2.1 concerning the correspondence or otherwise between the possible momentum operators for a particle confined to a finite interval of the real line and those for a particle constrained to move on a circle.

Let J be the interval $[0, 2\pi)$ in $\mathbb{R}$ and let S^1 be the unit circle $\{(\sin\theta, \cos\theta) : \theta \in J\}$ in $\mathbb{R}^2$. The state of a particle confined to J is assumed to be an element of the Hilbert space $\mathcal{H}(J) \equiv L^2(J)$ and the possible states of a particle on S^1 are assumed to be elements of $\mathcal{H}(S^1) \equiv L^2(S^1)$. Now, as is well known, there is no unique momentum operator for the interval. For instance if we start with the 'minimal operator' $\widehat{P}_o(J)$ defined on $C_o^\infty(J)$ by $\widehat{P}_o(J) = -i\hbar d/dx$, then $\widehat{P}_o(J)$ has the one-parameter family of self-adjoint extensions $\left\{\widehat{P}^\lambda(J) : \lambda \in (-\pi, \pi]\right\}$ where

$$\mathcal{D}\left(\widehat{P}^\lambda(J)\right) = \left\{\phi \in \mathcal{H}(J) : \phi \in AC(J), \phi' \in \mathcal{H}(J), \phi(0) = e^{-i\lambda}\phi(2\pi^-)\right\}$$

and

$$\widehat{P}^\lambda(J)\phi = -i\hbar\frac{d\phi}{d\theta} \quad \forall\phi \in D\left(\widehat{P}^\lambda(J)\right).$$

Note that the derivative $d/d\theta$ is well defined for all $\theta \in (0, 2\pi)$ in the usual manner. At

$\theta = 0$ however, $d/d\theta$ is understood to be defined in terms of a right hand limit. Clearly, this feature is not characteristic of a space like S^1. The problem is that S^1 is topologically distinct from J; though S^1 and J are isomorphic, they are not homeomorphic to one another [79, pp 232–233].

To define a global derivative on S^1 we must introduce (at least) two overlapping coordinate charts, say

$$\theta_1 \in (0, 2\pi) \quad \text{and} \quad \theta_2 \in (-\pi, \pi)$$

where the points $\theta_1 = 0^+$ and $\theta_2 = 0^+$ coincide with $\theta = 0^+$. Now consider the operator $\widehat{P}_o(S^1)$ defined on $C_o^\infty(S^1)$ by $\widehat{P}_o(S^1) = -i\hbar L$ where

$$L = \begin{cases} d/d\theta_1 & \theta_1 \in (0, 2\pi) \\ d/d\theta_2 & \theta_2 \in (-\pi, \pi). \end{cases}$$

Proposition: *The operator $\widehat{P}_o(S^1)$ defined above is essentially self-adjoint in $\mathcal{H}(S^1)$.*

Proof: Define the operator $\widehat{P}(S^1)$ on $AC(S^1)$ by $\widehat{P}(S^1) = -i\hbar L$. Let $\phi \in C_o^\infty(S^1)$ and $\psi \in AC(S^1)$, so

$$\begin{aligned} \langle \widehat{P}_o(S^1)\phi \mid \psi \rangle &= \int_{S^1} \left(\widehat{P}_o(S^1)\phi\right)^*(\theta)\psi(\theta)d\theta \\ &= \int_{0^+}^{2\pi^-} i\hbar \frac{d\phi^*}{d\theta_1}(\theta_1)\psi(\theta_1)d\theta_1 \\ &= i\hbar\left\{\phi^*(2\pi^-)\psi(2\pi^-) - \phi^*(0^+)\psi(0^+)\right\} \\ &\qquad -i\hbar\int_{0^+}^{2\pi^-} \phi^*(\theta_1)\frac{d\psi}{d\theta_1}(\theta_1)d\theta_1. \end{aligned} \tag{2.12}$$

Since $C_o^\infty(S^1) \subset AC(S^1)$ then $\phi(0^+) = \phi(2\pi^-)$ and $\psi(0^+) = \psi(2\pi^-)$, so the first term in RHS (2.12) vanishes and we are left with

$$\langle \widehat{P}_o(S^1)\phi \mid \psi \rangle = \langle \phi \mid \widehat{P}(S^1)\psi \rangle,$$

i.e.

$$\widehat{P}_o^\dagger(S^1) \supseteq \widehat{P}(S^1).$$

We now aim to show $\widehat{P}_o^\dagger(S^1) \subseteq \widehat{P}(S^1)$, and to do this it suffices to show $\mathcal{D}\left(\widehat{P}_o^\dagger(S^1)\right) \subseteq AC(S^1)$. Let ϕ be an element of $C_o^\infty(S^1)$, whose support is in $(0, 2\pi) \equiv J_o$, in particular we have

$$\phi(0) = \phi(0^+) = \phi(2\pi^-) = 0. \tag{2.13}$$

If $\psi \in \mathcal{D}\left(\widehat{P}_o^\dagger(S^1)\right)$ and $\psi_\sim \equiv \widehat{P}_o^\dagger(S^1)\psi$, then

$$\begin{aligned}
\langle \widehat{P}_o(S^1)\phi \mid \psi\rangle &= \langle \phi \mid \psi_\sim\rangle \\
&= \int_{0^+}^{2\pi^-} \phi^*(\theta_1)\psi_\sim(\theta_1)d\theta_1 \\
&= \int_{0^+}^{2\pi^-} \phi^*(\theta_1)\left\{\frac{d}{d\theta_1}\int_{0^+}^{\theta_1}\psi_\sim(\alpha)d\alpha + c\right\}d\theta_1,
\end{aligned}$$

where c is an arbitrary constant. Integrating by parts yields

$$\langle \widehat{P}_o(S^1)\phi \mid \psi\rangle = \phi^*(\theta_1)\left(\int_{0^+}^{\theta_1}\psi_\sim(\alpha)d\alpha + c\right)\Bigg|_{0^+}^{2\pi^-}$$

$$-\int_{0^+}^{2\pi^-}\left(\int_{0^+}^{\theta_1}\psi_\sim(\alpha)d\alpha + c\right)\frac{d\phi^*}{d\theta_1}(\theta_1)d\theta_1. \tag{2.14}$$

So now, via (2.13), we have

$$\int_{0^+}^{2\pi^-}\frac{d\phi^*}{d\theta_1}(\theta_1)\left\{i\hbar\psi(\theta_1) + \int_{0^+}^{\theta_1}\psi_\sim(\alpha)d\alpha + c\right\}d\theta_1 = 0, \tag{2.15}$$

and integrating by parts gives us

$$\int_{0^+}^{2\pi^-}\phi^*(\theta_1)\frac{d}{d\theta_1}\left\{i\hbar\psi(\theta_1) + \int_{0^+}^{\theta_1}\psi_\sim(\alpha)d\alpha + c\right\}d\theta_1 = 0,$$

where we have again used (2.13).

The set $C_o^\infty(J_o)$ is dense in $L^2(J_o)$ and since ϕ is, by assumption, an arbitrary element of $C_o^\infty(J_o)$ then

$$\frac{d}{d\theta_1}\left\{i\hbar\psi(\theta_1) + \int_{0^+}^{\theta_1}\psi_\sim(\alpha)d\alpha + c\right\}d\theta_1 = 0,$$

i.e.

$$\psi(\theta_1) = \frac{i}{\hbar}\int_{0^+}^{\theta_1}\psi_\sim(\alpha)d\alpha + k$$

where k is an arbitrary constant and it follows that $\psi(\theta)$ is absolutely continuous on $(0, 2\pi)$. To show that $\psi(\theta)$ is absolutely continuous on the whole of S^1 we may repeat the above analysis using the chart $\theta_2 \in (-\pi, \pi)$, i.e. consider instead $\phi(\theta_2)$ and $\psi(\theta_2)$. Hence $\psi \in AC(S^1)$ and $\widehat{P}_o^\dagger(S^1) = \widehat{P}(S^1)$.

The operator $\widehat{P}(S^1)$ is known to be self-adjoint [80]. It follows that $\widehat{P}_o(S^1)$ is essentially self-adjoint with unique self-adjoint extension $\widehat{P}(S^1)$ which coincides with the closure of $\widehat{P}_o(S^1)$ [42, p 96].

So, although there are uncountably many momentum operators associated with an interval, there is a single preferred choice for the momentum operator associated with a circle, namely $\widehat{P}(S^1)$. We can compare $\widehat{P}(S^1)$ with the various $\widehat{P}^\lambda(J)$s through the unitary groups they generate. Since $\widehat{P}(S^1)$ is self-adjoint in $\mathcal{H}(S^1)$ then $-i\widehat{P}(S^1)$ is the infinitesimal generator of a strongly continuous group $\{U_t : t \in \mathbb{R}\}$ of unitary operators on $\mathcal{H}(S^1)$ [58, pp 220–221]. This can be expressed formally as $U_t = exp\left(-it\widehat{P}(S^1)\right)$. The effect of U_t on an arbitrary element ϕ of $\mathcal{H}(S^1)$ is given by

$$(U_t\phi)(\theta) = \phi([\theta - t])$$

where $[\theta - t] \equiv (\theta - t)modulo(2\pi) \in [0, 2\pi)$. To see this, we note that locally U_t behaves like the familiar translation operator on $\mathbb{R}$ associated with the momentum operator $\widehat{P}$ in $L^2(\mathbb{R})$ [42, p 363]. Now since $\{U_t : t \in \mathbb{R}\}$ constitutes a group then for arbitrarily large t we can replace the action of U_t by a succession of local 'translations' $U_{t_1}U_{t_2}....$ such that $\sum_i t_i = t$. In particular if $t = 2n\pi$ then U_t coincides with the identity operator on $\mathcal{H}(S^1)$.

For the case of the interval, we also expect that the unitary group associated with $\widehat{P}^\lambda(J)$ behaves locally like the standard translation group on $\mathbb{R}$. In this case we have the added complication of what happens to the wavefunction near the endpoints of J.

Each $\lambda \in (-\pi, \pi]$ corresponds to a different momentum operator $\widehat{P}^\lambda(J)$ and so, by Stone's theorem, each λ is associated with a distinct unitary group. Let $\{U_t^\lambda : t \in \mathbb{R}\}$ denote the unitary group generated by $-i\widehat{P}^\lambda(J)$, then for arbitrary $\phi \in \mathcal{H}(J)$, we have

$$\left(U_t^\lambda\phi\right)(\theta) = e^{im\lambda}\phi([\theta - t]), \tag{2.16}$$

where m is an integer which satisfies $2\pi m = (\theta - t) - [\theta - t]$.

To prove this, we will use the relation [58, pp 220–222]:

$$U_t^\lambda = \int_{-\infty}^{\infty} e^{-it\mu} d_\mu \widehat{E}\left(\widehat{P}^\lambda(J); \mu\right).$$

Consider an eigenfunction ϕ_n^λ of $\widehat{P}^\lambda(J)$, where

$$\phi_n^\lambda(\theta) = \frac{1}{\sqrt{2\pi}} e^{\frac{i}{\hbar} P_n^\lambda \theta}; \qquad P_n^\lambda = (2\pi n + \lambda)\frac{\hbar}{2\pi}.$$

Now

$$\int_{-\infty}^{\infty} e^{-\frac{i}{\hbar} t\mu} d_\mu \widehat{E}\left(\widehat{P}^\lambda(J);\mu\right)\phi_n^\lambda(\theta) = e^{-\frac{i}{\hbar} tP_n^\lambda}\phi_n^\lambda(\theta) = \frac{1}{\sqrt{2\pi}} e^{\frac{i}{\hbar}\frac{\hbar}{2\pi}(2\pi n+\lambda)(\theta - t)}$$

$$= e^{\frac{i}{\hbar}\frac{\hbar}{2\pi}(2\pi n+\lambda)((\theta-t)-[\theta-t])}\frac{1}{\sqrt{2\pi}} e^{\frac{i}{\hbar}\frac{\hbar}{2\pi}(2\pi n+\lambda)([\theta-t])} = e^{im\lambda}\phi_n^\lambda\left([\theta - t]\right)$$

where $2\pi m = (\theta - t) - [\theta - t]$.

We have thus shown

$$\left(U_t^\lambda \phi_n^\lambda\right)(\theta) = e^{im\lambda}\phi_n^\lambda\left([\theta - t]\right) \tag{2.17}$$

where $2\pi m = (\theta - t) - [\theta - t]$, and since $\{\phi_n^\lambda : n = 0, \pm 1, \pm 2, ...\}$ is a basis for $\mathcal{H}(J)$ and U_t^λ is a continuous operator for all $t \in I\!R$ then (2.17) implies (2.16).

We see that wavefunctions which are translated by the action of U_t^λ beyond $\theta = 2\pi^-$ reappear at $\theta = 0$ modified by a phase factor $e^{i\lambda}$. In particular $U_{2n\pi}^\lambda$ is the identity on $\mathcal{H}(J)$ if and only if $\lambda = 0$.

Appendix H: Direct Integrals and Maximal Symmetric Operators

Let $\mathcal{H}(\lambda)$ be a one parameter family of Hilbert spaces for which we can define a direct integral Hilbert space $\mathcal{H}^{\oplus}$ by

$$\mathcal{H}^{\oplus} = \int_{\mathbb{R}}^{\oplus} \mathcal{H}(\lambda) d\mu(\lambda)$$

where $\mu(\lambda)$ is an appropriate generating function of some Lebesgue - Stieltjes measure [22, pp 455–456].[4]

Let $\widehat{A}(\lambda)$ be a measurable function defined on the real line, which assigns to each $\lambda \in \mathbb{R}$ a maximal symmetric operator with deficiency indices $(n_+, n_-) = (n, 0)$, defined in the Hilbert space $\mathcal{H}(\lambda)$.

Define the operator $\widehat{A}^{\oplus}$ in $\mathcal{H}^{\oplus}$ on the domain

$$\mathcal{D}(\widehat{A}^{\oplus}) = \left\{ \phi^{\oplus} \in \mathcal{H}^{\oplus} : \phi(\lambda) \in \mathcal{D}\left(\widehat{A}(\lambda)\right) a.e., \int_{\mathbb{R}} \left\| \widehat{A}(\lambda)\phi(\lambda) \right\|_{\lambda}^{2} d\mu(\lambda) < \infty \right\}$$

by

$$\left(\widehat{A}^{\oplus}\phi^{\oplus}\right)(\lambda) = \widehat{A}(\lambda)\phi(\lambda).$$

This can be expressed symbolically by writing

$$\widehat{A}^{\oplus} = \int_{\mathbb{R}}^{\oplus} \widehat{A}(\lambda) d\mu(\lambda).$$

We can show that if $\left(\widehat{A}(\lambda) + i\right)^{-1}$ is a measurable function then $\widehat{A}^{\oplus}$ is maximal symmetric.

[4] For the case where $\mu(\lambda)$ is a discrete measure, the direct integral reduces to a direct sum.

Reed and Simon [65, pp 283–284] have proved this for the case where all the $\mathcal{H}(\lambda)$ are the same and where $\widehat{A}(\lambda)$ is a self-adjoint operator valued function, indeed $\widehat{A}^{\oplus}$ is self-adjoint. We shall relax these requirements and show that the derivation still carries through.

Note that our analysis can also be applied to those $\widehat{A}(\lambda)$ which assign to each λ a maximal symmetric operator in $\mathcal{H}(\lambda)$ with $n_+ = 0$. Since if, for fixed λ, $\widehat{A}(\lambda)$ is maximal symmetric in $\mathcal{H}(\lambda)$ with deficiency indices $(0, n)$ then $-\widehat{A}(\lambda)$ is maximal symmetric with deficiency indices $(n, 0)$ (appendix A), so we would just consider the function $-\widehat{A}(\lambda)$ instead.

Since $n_- = 0$ for all $\widehat{A}(\lambda)$ then the range of $(\widehat{A}(\lambda) + i)$, denoted $\mathcal{R}(\widehat{A}(\lambda) + i)$, coincides with $\mathcal{H}(\lambda)$. We now aim to show $\mathcal{R}(\widehat{A}^{\oplus} + i) = \mathcal{H}^{\oplus}$.

Firstly, since for fixed λ, $\widehat{A}(\lambda)$ is symmetric with $n_- = 0$, then $\widehat{A}(\lambda) + i$ is invertible and $\widehat{C}(\lambda) \equiv \left(\widehat{A}(\lambda) + i\right)^{-1}$ is bounded with bound not exceeding 1 [58, pp 98,107], [81, p 270].

By assumption, $\widehat{C}(\lambda)$ is measurable and we may define $\widehat{C}^{\oplus} = \int_{\mathbb{R}}^{\oplus} \widehat{C}(\lambda) d\mu(\lambda)$ on $\mathcal{H}^{\oplus}$.

Let $\psi^{\oplus} = \widehat{C}^{\oplus} \eta^{\oplus}$ for an arbitrary $\eta^{\oplus} \in \mathcal{H}^{\oplus}$.

Since $\mathcal{R}\left(\widehat{A}(\lambda) + i\right) = \mathcal{H}(\lambda)$, i.e. for arbitrary $\xi(\lambda) \in \mathcal{H}(\lambda)$ there exists a $\phi(\lambda) \in \mathcal{D}\left(\widehat{A}(\lambda)\right)$ such that a.e.

$$\left(\widehat{A}(\lambda) + i\right) \phi(\lambda) = \xi(\lambda),$$

then

$$\phi(\lambda) = \widehat{C}(\lambda) \xi(\lambda),$$

so the range of $\widehat{C}(\lambda)$ is $\mathcal{D}\left(\widehat{A}(\lambda)\right)$.

Now [81, p 270],

$$\left\| \left(\widehat{A}(\lambda) + i\right) \left(\widehat{A}(\lambda) + i\right)^{-1} \eta(\lambda) \right\|_{\lambda}^{2} = \left\| \widehat{A}(\lambda) \left(\widehat{A}(\lambda) + i\right)^{-1} \eta(\lambda) \right\|_{\lambda}^{2} + \left\| \left(\widehat{A}(\lambda) + i\right)^{-1} \eta(\lambda) \right\|_{\lambda}^{2},$$

therefore

$$\left\| \widehat{A}(\lambda) \widehat{C}(\lambda) \eta(\lambda) \right\|_{\lambda}^{2} = \|\eta(\lambda)\|_{\lambda}^{2} - \left\| \widehat{C}(\lambda) \eta(\lambda) \right\|_{\lambda}^{2},$$

so

$$\left\|\widehat{A}(\lambda)\psi(\lambda)\right\|_{\lambda} \leq \|\eta(\lambda)\|_{\lambda}.$$

Hence $\psi^{\oplus} \in \mathcal{D}(\widehat{A}^{\oplus})$ and since a.e.

$$\left(\widehat{A}(\lambda)+i\right)\psi(\lambda)=\eta(\lambda),$$

then we have

$$(\widehat{A}^{\oplus}+i)\psi^{\oplus}=\eta^{\oplus}.$$

So

$$\mathcal{R}(\widehat{A}^{\oplus}+i)=\mathcal{H}^{\oplus}.$$

It follows that $\widehat{A}^{\oplus}$ is maximal symmetric [58, pp 230–233,239].

Chapter 3

QUANTISATION AND FUNCTIONS OF MAXIMAL SYMMETRIC OPERATORS

It is not only the idempotency and orthogonality of its spectral function which sets apart the self-adjoint operator from the more general maximal symmetric operator. It is relatively straightforward to define a function of a self-adjoint operator which is also self-adjoint. This property is particularly useful when applied to the quantisation of a function of a classical observable. Also, self-adjoint operators, and only self-adjoint operators, can be used to generate (strongly) continuous groups of unitary operators. Such unitary groups have an important role in orthodox quantum mechanics, especially in relation to the temporal evolution of a quantum system.

In this chapter, we consider the possibility of extending the notion of function of a self-adjoint operator to encompass all maximal symmetric operators. We shall also examine the appropriate generalisation of unitary groups for which maximal symmetric operators are the generators; this entails the study of isometric semigroups.

3.1 Orthodox Observables and Functions of Self-Adjoint Operators

If f is a real (Borel) measurable function on $\mathbb{R}$ and $\widehat{A}$ is a self-adjoint operator defined in a Hilbert space $\mathcal{H}$ then $f(\widehat{A})$ is defined by

$$\mathcal{D}\left(f(\widehat{A})\right) = \left\{\phi \in \mathcal{H} : \int_{\mathbb{R}} |f(\lambda)|^2 d_\lambda \langle \phi \mid \widehat{E}(\widehat{A};\lambda)\phi\rangle < \infty\right\}$$

and

$$\langle \psi \mid f(\widehat{A})\phi\rangle = \int_{\mathbb{R}} f(\lambda) d_\lambda \langle \psi \mid \widehat{E}(\widehat{A};\lambda)\phi\rangle \;\; \forall \phi \in \mathcal{D}\left(f(\widehat{A})\right),\; \psi \in \mathcal{H}, \tag{3.1}$$

where $f(\widehat{A})$ is self-adjoint in $\mathcal{H}$ [57, pp 263–264].

The spectral measure of $f(\widehat{A})$ is given by [55, pp 1196,1200–1201]

$$\widehat{E}\left(f(\widehat{A});\Lambda\right) = \widehat{E}\left(\widehat{A};f^{-1}(\Lambda)\right) \tag{3.2}$$

where Λ is an arbitrary Borel set.

It is clear from eqn (3.2) that $f(\widehat{A})$ defined in this way can be interpreted as a rescaling of the measuring device used to measure the observable represented by $\widehat{A}$.

We shall see shortly that the relations akin to (3.1) and (3.2) for general maximal symmetric operators are incompatible. The implications of this with regard to observables being represented by non-self-adjoint maximal symmetric operators are considered.

3.2 The Square of a Maximal Symmetric Operator

Suppose a classical observable A is quantised to yield a maximal symmetric operator $\widehat{A}$. If $\widehat{A}$ is self-adjoint then $\widehat{A}^2$ as defined above is also self-adjoint and is therefore a candidate for the quantised version of the classical observable A^2. On the other hand, if $\widehat{A}$ is not self-adjoint then we do not necessarily have that $\widehat{A}^2$ is maximal symmetric. For example consider the momentum operator $\widehat{P}_+$ for a particle confined to $\boldsymbol{R}^+$ (appendix A). Squaring $\widehat{P}_+$ yields

$$\mathcal{D}(\widehat{P}_+^2) = \left\{\phi \in \mathcal{D}(\widehat{P}_+) : \phi' \in \mathcal{D}(\widehat{P}_+)\right\}$$

$$= \left\{\phi \in L^2(\mathbb{R}^+) : \phi, \phi' \in AC(\mathbb{R}^+), \phi', \phi'' \in L^2(\mathbb{R}^+), \phi(0) = \phi'(0) = 0\right\}$$

and

$$\widehat{P}_+^2\phi = -\hbar^2 \frac{d^2\phi}{dx^2} \quad \forall \phi \in \mathcal{D}(\widehat{P}_+^2).$$

It is clear that $\widehat{P}_+^2$ is a proper restriction of the operator $\widehat{P}_+^\dagger \widehat{P}_+$, which acts on the larger domain

$$\mathcal{D}(\widehat{P}_+^\dagger \widehat{P}_+) = \left\{\phi \in \mathcal{D}(\widehat{P}_+) : \phi' \in \mathcal{D}(\widehat{P}_+^\dagger)\right\},$$

i.e. the derivative of states in $\mathcal{D}(\widehat{P}_+^\dagger \widehat{P}_+)$ need not vanish at the origin. It turns out that $\widehat{P}_+^\dagger \widehat{P}_+$ is self-adjoint, it is called the Friedrichs extension of $\widehat{P}_+^2$ [50, p 181]. Hence $\widehat{P}_+^2$ is not maximal symmetric.

Let $\widehat{A}$ be an arbitrary maximal symmetric operator. Now $\widehat{A}^\dagger \widehat{A}$ is self-adjoint where $\mathcal{D}(\widehat{A}^\dagger \widehat{A}) = \{\phi \in \mathcal{D}(\widehat{A}) : \widehat{A}\phi \in \mathcal{D}(\widehat{A}^\dagger)\}$. For $\psi \in \mathcal{D}(\widehat{A})$ and $\phi \in \mathcal{D}(\widehat{A}^\dagger \widehat{A})$, we have the following:

$$\langle \psi \mid \widehat{A}^\dagger \widehat{A}\phi \rangle = \langle \widehat{A}\psi \mid \widehat{A}\phi \rangle = \int_{-\infty}^{\infty} \lambda d_\lambda \langle \widehat{A}\psi \mid \widehat{F}(\widehat{A}; \lambda)\phi \rangle.$$

Now from [11, p 133],[1] the following relation holds for all $\psi, \phi \in \mathcal{D}(\widehat{A})$:

$$\langle \widehat{A}\psi \mid \widehat{F}(\widehat{A}; \lambda)\phi \rangle = \int_{-\infty}^{\lambda} \lambda' d_{\lambda'} \langle \psi \mid \widehat{F}(\widehat{A}; \lambda')\phi \rangle.$$

[1]Note that equation (11) in [11, p 133] also holds for non-finite Δ.

So

$$\begin{aligned}\langle \widehat{A}\psi \mid \widehat{A}\phi\rangle &= \int_{-\infty}^{\infty} \lambda d_\lambda \int_{-\infty}^{\lambda} \lambda' d_{\lambda'} \langle \psi \mid \widehat{F}(\widehat{A};\lambda')\phi\rangle \\ &= \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \psi \mid \widehat{F}(\widehat{A};\lambda)\phi\rangle\end{aligned}$$

and as $\mathcal{D}(\widehat{A})$ is dense we have

$$\langle \psi \mid \widehat{A}^\dagger\widehat{A}\phi\rangle = \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \psi \mid \widehat{F}(\widehat{A};\lambda)\phi\rangle \ \ \forall \psi \in \mathcal{H}, \phi \in \mathcal{D}(\widehat{A}^\dagger\widehat{A}).$$

So $\widehat{A}^\dagger\widehat{A}$ can be expressed in a similar fashion to the square of a self-adjoint operator, i.e. eqn (3.1).

There are other extensions of $\widehat{A}^2$. Take $\widehat{A}\widehat{A}^\dagger$ for instance. Since $\widehat{A}$ is maximal symmetric then $\widehat{A}$ is closed and $(\widehat{A}^\dagger)^\dagger = \widehat{A}$, so $\widehat{A}\widehat{A}^\dagger = (\widehat{A}^\dagger)^\dagger\widehat{A}^\dagger$ and it follows [50, p 180] that $\widehat{A}\widehat{A}^\dagger$ is self-adjoint. Note that generally we do not have $\widehat{A}\widehat{A}^\dagger = \widehat{A}^\dagger\widehat{A}$, i.e. maximal symmetric operators need not be normal. Compare $\widehat{P}_+^\dagger\widehat{P}_+$ and $\widehat{P}_+\widehat{P}_+^\dagger$, for $\phi \in \mathcal{D}(\widehat{P}_+^\dagger\widehat{P}_+)$, we must have $\phi(0) = 0$ but not necessarily that $\phi'(0) = 0$ whereas for $\psi \in \mathcal{D}(\widehat{P}_+\widehat{P}_+^\dagger)$, we must have $\psi'(0) = 0$ but we do not require $\psi(0) = 0$.

While, mathematically, the Friedrichs extension has many attractive properties, some of which are unique to it ([50, pp 177–179], [81, pp 325–326]), the only characteristic which is desirable from a physical viewpoint is that the lower bounds of $\widehat{A}^\dagger\widehat{A}$ and $\widehat{A}^2$ coincide. However, there are extensions other than the Friedrichs extension which also share this property. In the next section we give an example of where the Friedrichs extension *is* singled out as the preferred choice of extension.

3.2.1 The Friedrichs Extension and the Radial Part of the Free Hamiltonian in Spherical Polar Coordinates

The main reference for this section is [50, pp 160–161].

Our starting point is the operator $\widehat{H}_o$ defined in

$$L^2(\mathbb{R}^3) = L^2(\mathbb{R}^+, r^2dr) \otimes L^2(S^2, \sin\theta d\theta d\varphi)$$

on domain

$$\mathcal{D}(\widehat{H}_o) = C_o^\infty(\mathbb{R}_o^3)$$

by

$$\widehat{H}_o\psi = -\frac{\hbar^2}{2m}\nabla^2\psi \ \ \forall\psi \in \mathcal{D}(\widehat{H}_o),$$

where $\mathbb{R}_o^3$ denotes the set $\mathbb{R}^3$ with the origin removed and

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial\psi}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial\psi}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}.$$

The operator

$$-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$$

defined on $C^\infty(S^2)$ is essentially self-adjoint in $L^2(S^2)$ and has a purely discrete spectrum [50, p 160]. We denote by K_l the eigenspace corresponding to its lth eigenvalue λ_l ($l \geq 0$). So, as is well known, K_l is spanned by the spherical harmonics $Y_l^m(\theta,\varphi)$ where $-l \leq m \leq l$ and $\lambda_l = \hbar^2 l(l+1)$ [82, pp 176–185].

Next consider the set of functions in $\mathcal{D}(\widehat{H}_o)$ which are linear combinations of those $\psi(r,\theta,\varphi)$ of the form $\phi(r)\xi(\theta,\varphi)$. This set, denoted $\overline{\mathcal{D}}$, is dense in $L^2(\mathbb{R}^3)$. We now decompose $L^2(\mathbb{R}^3)$ thus

$$L^2(\mathbb{R}^3) = \oplus_{l=0}^{\infty}L_l$$

where

$$L_l = L^2(\mathbb{R}^+, r^2dr) \otimes K_l.$$

Define $\mathcal{D}_l = \overline{\mathcal{D}} \cap L_l$, then the restriction of $\widehat{H}_o$ to $\mathcal{D}_l$ is given by

$$\widehat{H}_o|_{\mathcal{D}_l} = \left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{l(l+1)\hbar^2}{2mr^2}\right) \otimes \widehat{I}.$$

Now $\widehat{H}_o$ is essentially self-adjoint on $\mathcal{D}(\widehat{H}_o)$ if and only if the operator $\widehat{h}_o$, defined by

$$\widehat{h}_o \equiv -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{l(l+1)\hbar^2}{2mr^2},$$

is essentially self-adjoint on $C_o^\infty(\mathbb{R}_o^+)$ [50, p 161].

We can simplify matters by making use of the unitary map $\widehat{U}$ between $L^2(\mathbb{R}^+, r^2dr)$ and $L^2(\mathbb{R}^+, dr)$ defined by

$$\widehat{U}\phi = \phi_\sim = r\phi \in L^2(\mathbb{R}^+, dr) \ \ \forall\phi \in L^2(\mathbb{R}^+, r^2dr)$$

and

$$\widehat{U}^{-1}\phi_\sim = \phi = \frac{\phi_\sim}{r} \in L^2(\mathbb{R}^+, r^2dr) \;\; \forall \phi_\sim \in L^2(\mathbb{R}^+, dr).$$

Hereafter a tilde is used to identify functions and operators associated with $L^2(\mathbb{R}^+, dr)$.

Transforming $\widehat{h}_o$, we have

$$\begin{aligned} \widehat{h}_{o_\sim} &\equiv \widehat{U}\widehat{h}_o\widehat{U}^{-1} \\ &= -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} \end{aligned}$$

defined on $C_o^\infty(\mathbb{R}_o^+)$ in $L^2(\mathbb{R}^+, dr)$.

The operator $\widehat{h}_{o_\sim}$ has the familiar form of a one-dimensional Hamiltonian describing a particle constrained to move in $\mathbb{R}_o^+$ under the influence of the 'centrifugal potential'

$$V(r) = \frac{l(l+1)\hbar^2}{2mr^2}.$$

Now from [50, p 161], $\widehat{h}_{o_\sim}$ is essentially self-adjoint if and only if $l(l+1) \geq 3/4$. Clearly the only non essentially self-adjoint $\widehat{h}_{o_\sim}$ is given by $l = 0$, i.e. for zero angular momentum (the same is true in two dimensions). In this instance the deficiency indices of $\widehat{h}_{o_\sim}$ are $(1,1)$ and there is a one-parameter family of self-adjoint extensions, each extension being identified by a particular boundary condition at the origin.

For $l \neq 0$, $\widehat{h}_{o_\sim}$ is essentially self-adjoint so we do not need to impose a boundary condition and its only self-adjoint extension is its closure. In this case the potential $l(l+1)\hbar^2/2mr^2$ is said to be quantum mechanically complete [50, p 154].

So, for $l = 0$, we need to choose a particular self-adjoint extension of

$$\widehat{h}_{o_\sim} = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} \;\text{ on }\; C_o^\infty(\mathbb{R}_o^+) \;\text{ in }\; L^2(\mathbb{R}^+, dr).$$

The various self-adjoint extensions of $\widehat{h}_{o_\sim}$ are characterised thus [50, p 144]:

$$\mathcal{D}(\widehat{h}_\sim^{(a)}) = \left\{\phi_\sim \in L^2(\mathbb{R}^+, dr) : \phi'_\sim \in AC(\mathbb{R}_o^+), \phi''_\sim \in L^2(\mathbb{R}^+, dr), \phi'_\sim(0^+) + a\phi_\sim(0^+) = 0\right\}$$

$$\mathcal{D}(\widehat{h}_\sim^{(\infty)}) = \left\{\phi_\sim \in L^2(\mathbb{R}^+, dr) : \phi'_\sim \in AC(\mathbb{R}_o^+), \phi''_\sim \in L^2(\mathbb{R}^+, dr), \phi_\sim(0^+) = 0\right\},$$

where all extensions act on their respective domains as $-(\hbar^2/2m)d^2/dr^2$.

Next consider the non-self-adjoint maximal symmetric operator $\widehat{P}^+_\sim$ defined on

$$\mathcal{D}(\widehat{P}^+_\sim) = \left\{\phi_\sim \in L^2(\mathbb{R}^+, dr) : \phi_\sim \in AC(\mathbb{R}^+_o), \phi'_\sim \in L^2(\mathbb{R}^+, dr), \phi_\sim(0^+) = 0\right\}$$

by

$$\widehat{P}^+_\sim = -i\hbar\frac{d}{dr}.$$

The adjoint of $\widehat{P}^+_\sim$ is defined on

$$\mathcal{D}\left((\widehat{P}^+_\sim)^\dagger\right) = \left\{\phi_\sim \in L^2(\mathbb{R}^+, dr) : \phi_\sim \in AC(\mathbb{R}^+_o), \phi'_\sim \in L^2(\mathbb{R}^+, dr)\right\}$$

by

$$(\widehat{P}^+_\sim)^\dagger = -i\hbar\frac{d}{dr}.$$

The operators $(\widehat{P}^+_\sim)^\dagger\widehat{P}^+_\sim$ and $\widehat{P}^+_\sim(\widehat{P}^+_\sim)^\dagger$ defined respectively on

$$\mathcal{D}\left((\widehat{P}^+_\sim)^\dagger\widehat{P}^+_\sim\right) = \left\{\phi_\sim \in \mathcal{D}(\widehat{P}^+_\sim) : \widehat{P}^+_\sim\phi_\sim \in \mathcal{D}\left((\widehat{P}^+_\sim)^\dagger\right)\right\}$$

and

$$\mathcal{D}\left(\widehat{P}^+_\sim(\widehat{P}^+_\sim)^\dagger\right) = \left\{\phi_\sim \in \mathcal{D}\left((\widehat{P}^+_\sim)^\dagger\right) : (\widehat{P}^+_\sim)^\dagger\phi_\sim \in \mathcal{D}(\widehat{P}^+_\sim)\right\}$$

act on their respective domains as $-(\hbar^2/2m)d^2/dr^2$ and are both self-adjoint extensions of $\widehat{h}_{o_\sim}$.

That they are extensions of $\widehat{h}_{o_\sim}$ is obvious, that they are self-adjoint extensions follows from the result that if $\widehat{A}$ is an arbitrary closed densely defined operator then $\widehat{A}^\dagger\widehat{A}$ is self-adjoint and in particular, for maximal symmetric $\widehat{A}$, $\widehat{A}\widehat{A}^\dagger = (\widehat{A}^\dagger)^\dagger\widehat{A}^\dagger$, so $\widehat{A}\widehat{A}^\dagger$ is also self-adjoint (cf. previous section).

Since every $\phi_\sim \in \mathcal{D}\left((\widehat{P}^+_\sim)^\dagger\widehat{P}^+_\sim\right)$ satisfies $\phi_\sim(0^+) = 0$ then it follows that $\widehat{h}^{(\infty)}_\sim = (\widehat{P}^+_\sim)^\dagger\widehat{P}^+_\sim$. Likewise since every $\phi_\sim \in \mathcal{D}\left(\widehat{P}^+_\sim(\widehat{P}^+_\sim)^\dagger\right)$ satisfies $\phi'_\sim(0^+) = 0$ then it follows that $\widehat{h}^{(o)}_\sim = \widehat{P}^+_\sim(\widehat{P}^+_\sim)^\dagger$.

Generalised Eigenfunctions

The generalised eigenfunctions of any of the self-adjoint extensions of $\widehat{h}_{o_\sim}$ are solutions of the equation

$$\frac{d^2\psi^k_\sim}{dr^2} + k^2\psi^k_\sim = 0.$$

These are of the form

$$\underset{\sim}{\psi}^k(r) = \alpha_1 \frac{\sin(kr)}{k} - \alpha_2 \frac{\cos(kr)}{k} \tag{3.3}$$

where α_1 and α_2 are arbitrary complex numbers.

We have seen that each of the various $\underset{\sim}{\widehat{h}}^{(a)}$ is identified by a boundary condition

$$\underset{\sim}{\phi}'(0^+) = -a\underset{\sim}{\phi}(0^+).$$

Now, $\underset{\sim}{\psi}^k$ satisfies this boundary condition provided

$$a = \frac{\alpha_1}{\alpha_2} k.$$

For example, the case $a = 0$ corresponds to $\alpha_1 = 0$ and the case $a = \infty$ corresponds to $\alpha_2 = 0$.

For $\alpha_1 = 0$,

$$\underset{\sim}{\psi}^k(r) \sim \frac{\cos(kr)}{k},$$

or

$$\psi^k(r) \sim n_o(kr)$$

where $n_o(kr)$ is the zeroth order Neumann function $-(1/kr)\cos(kr)$ [82, p 197], [83, pp 297–299].

For $\alpha_2 = 0$,

$$\underset{\sim}{\psi}^k(r) \sim \frac{\sin(kr)}{k},$$

or

$$\psi^k(r) \sim j_o(kr)$$

where $j_o(kr)$ is the zeroth order spherical Bessel function $(1/kr)\sin(kr)$ (ref. ibid.).

The preferred choice of boundary condition inferred from textbook treatments (see for example [23, pp 155–156], [82, pp 194–197] and [83, pp 170,297]) is such as to exclude those solutions which are singular at the origin. Clearly as $r \to 0$, $n_o(kr)$ behaves like $1/r$, so α_2 is chosen to be zero. The appropriate extension is then $\underset{\sim}{\widehat{h}}^{(\infty)} = (\underset{\sim}{\widehat{P}}^+)^\dagger \underset{\sim}{\widehat{P}}^+$ which, as we know, is just the Friedrichs extension of $(\underset{\sim}{\widehat{P}}^+)^2$.

Within the context of orthodox quantum mechanics it is generally assumed that if a classical observable A is quantised to give a self-adjoint operator $\widehat{A}$ then the classical observable A^2 should be quantised as $\widehat{A}^2$, which is also self-adjoint. As we have seen, application of this correspondence rule to the case where A is quantised as a non-self-adjoint maximal symmetric operator does not necessarily yield an acceptable quantised A^2, i.e. $\widehat{A}^2$ may not be maximal symmetric. In this instance we will have to choose a particular maximal symmetric extension of $\widehat{A}^2$ and this will depend on physical considerations. Note that there is no more ambiguity here than in choosing the particular $\widehat{A}$ to represent the quantum mechanical counterpart of A in the first place.

Let $\widehat{B}$ be a maximal symmetric extension of $\widehat{A}^2$, where $\widehat{A}$ is maximal symmetric. Since $\widehat{A}^2$ is positive then $\widehat{B}$ is self-adjoint [50, p 177: thm X.23] and therefore possesses a unique orthogonal spectral function. Now unless $\widehat{A}$ is self-adjoint, we generally do not have

$$\widehat{F}(\widehat{B};\Lambda) = \widehat{F}(\widehat{A};\sqrt{\Lambda})$$

since the LHS is a projector whereas the RHS need not be. However, on $\mathcal{D}(\widehat{A})$ we do have

$$\langle\phi \mid \widehat{B}\phi\rangle = \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle\phi \mid \widehat{F}(\widehat{A};\lambda)\phi\rangle$$

and we thus see the inequivalence of (3.1) and (3.2) when extended to our generalised theory. So, by allowing an arbitrary maximal symmetric operator $\widehat{A}$ to represent an observable, we generally cannot interpret $f(\widehat{A})$, as defined by a relation analogous to (3.1), in terms of a rescaling of the measuring device. In other words, measurement of $f(\widehat{A})$ would not be described by the POV measure $\widehat{F}\big(\widehat{A};f^{-1}(\Lambda)\big)$. Of course, if the measuring device *is* rescaled and this rescaling is characterised by f then $f(\widehat{A})$ should be defined in terms of the POV measure $\widehat{F}\big(\widehat{A};f^{-1}(\Lambda)\big)$. We would then interpret $\widehat{F}\big(\widehat{A};f^{-1}(\Lambda)\big)$ as an adapted observable (chapter 2) which takes into account the rescaling of the measuring device used to measure observable $\widehat{A}$.

3.3 Higher Powers

We note from the above that although $\widehat{A}^2$ is maximal symmetric if $\widehat{A}$ is self-adjoint, we do not necessarily have that $\widehat{A}^2$ is maximal symmetric for arbitrary maximal symmetric $\widehat{A}$. In fact the following is true [58, pp 108–109,239,243]:

Theorem 13 *If $\widehat{A}$ is a closed symmetric operator then $\widehat{A}^N$, for $N > 1$, is maximal symmetric if and only if $\widehat{A}$ is self-adjoint.*

If $\widehat{A}$ is a non-self-adjoint maximal symmetric operator, theorem 13 tells us that $\widehat{A}^N$ will not be maximal symmetric and we are forced to seek an appropriate maximal symmetric extension assuming one exists. In practice though, the operator $\widehat{A}^N$ would be redefined on as small a dense domain as possible. This would generate, through its maximal symmetric extensions, a larger selection of candidate observables for the quantised A^N. Here, we shall consider the specific example of positive integer powers of the half-line momentum $\widehat{P}_+$ (appendix A), or rather the existence and nature of any maximal symmetric extensions of the operator $\widehat{T}_{n,o}$ (the notation is that of Weidmann [58, § 6.4]) which is defined by

$$\mathcal{D}(\widehat{T}_{n,o}) = C_o^\infty(\mathbb{R}^+)$$

and

$$\widehat{T}_{n,o}\phi = (-i)^n \frac{d^n\phi}{dx^n} \quad \forall\phi \in \mathcal{D}(\widehat{T}_{n,o}),$$

where $\widehat{T}_{n,o}$ is symmetric with adjoint $\widehat{T}_{n,o}^\dagger$ defined by [58, p 160: thm 6.29]

$$\mathcal{D}(\widehat{T}_{n,o}^\dagger) = \{\phi \in L^2(\mathbb{R}^+) : \phi, \phi', \phi'', \ldots, \phi^{(n-2)} \text{ continuously differentiable on } \mathbb{R}^+,$$

$$\phi^{(n-1)} \in AC(\mathbb{R}^+), \phi^{(n)} \in L^2(\mathbb{R}^+)\}$$

and

$$\widehat{T}_{n,o}^\dagger\phi = (-i)^n \frac{d^n\phi}{dx^n} \quad \forall\phi \in \mathcal{D}(\widehat{T}_{n,o}^\dagger).$$

If n is even then $\widehat{T}_{n,o}$ is positive and so all of its maximal symmetric extensions will be self-adjoint [58, p 163]. To determine the nature of the maximal symmetric extensions for n odd we shall find the deficiency indices of $\widehat{T}_{n,o}$.

The deficiency indices (n_+, n_-) of $\widehat{T}_{n,o}$ are given by the number of linearly independent solutions, which lie in $\mathcal{D}(\widehat{T}^\dagger_{n,o})$, of the equations

$$(-i)^n \frac{d^n\phi}{dx^n} = i\phi$$

and

$$(-i)^n \frac{d^n\phi}{dx^n} = -i\phi$$

respectively (appendix A).

Firstly we consider n of the form $4l+1$ where $l = 0, 1, 2, \ldots$. Here, n_+ is determined by the equation

$$-\frac{d^n\phi}{dx^n} = \phi \tag{3.4}$$

and n_- by the equation

$$\frac{d^n\phi}{dx^n} = \phi. \tag{3.5}$$

All other odd n are of the form $4l+3$, $l = 1, 2, \ldots$, and for such n equations (3.4) and (3.5) are interchanged.

Solutions of the equations $d^n\phi/dx^n = \pm\phi$ can be obtained by elementary methods [84, p 73], i.e. we subst $\phi = exp(mx)$, to obtain $m^n = \pm 1$. Now the set of nth roots of 1 and -1 are

$$\left\{\cos\left(\frac{k2\pi}{n}\right) + i\sin\left(\frac{k2\pi}{n}\right)\right\}$$

and

$$\left\{\cos\left(\frac{(k+1/2)2\pi}{n}\right) + i\sin\left(\frac{(k+1/2)2\pi}{n}\right)\right\}$$

respectively, where $k = 0, 1, 2, \ldots, (n-1)$ [84, p 12].

We shall be interested in those roots which have a negative real part. For a real number $\theta \in [0, 1)$, we have

$$\cos(2\pi\theta) < 0 \text{ if and only if } \frac{1}{4} < \theta < \frac{3}{4}.$$

Clearly $exp(mx) \in \mathcal{D}(\widehat{T}^\dagger_{n,o})$ if and only if $exp(mx) \in L^2(\mathbb{R}^+)$ and the only relevant part of the root which determines whether or not $exp(mx) \in L^2(\mathbb{R}^+)$ is the real part. We consider first $n = 4l+1$ only. For n_- we have $\theta = k/n$ and for n_+, $\theta = (k+1/2)/n$. We now show that $n_+ = n_- + 1$. Firstly we have $n_+ \geq n_-$, which is clear from the following two propositions:

$$(i) \quad \frac{1}{4} < \frac{k}{n} \Longrightarrow \frac{1}{4} < \frac{k+\frac{1}{2}}{n},$$
$$(ii) \quad \frac{k}{n} < \frac{3}{4} \Longrightarrow \frac{k+\frac{1}{2}}{n} < \frac{3}{4}.$$

Proposition (i) is obvious. To prove (ii) we have

$$\begin{aligned} 4k < 3n \quad &\Longrightarrow \quad 4k < 12l + 3 \\ &\Longrightarrow \quad k < 3l + \frac{3}{4} \\ &\Longrightarrow \quad k < 3l + \frac{1}{4} \\ &\Longrightarrow \quad \frac{k+\frac{1}{2}}{n} < \frac{3}{4}. \end{aligned}$$

That $n_+ > n_-$ follows from

$$(iii) \quad \frac{1}{4} < \frac{k+1}{n} \Longrightarrow \frac{1}{4} < \frac{k+\frac{1}{2}}{n}.$$

To prove (iii), we have

$$\begin{aligned} n < 4k + 4 \quad &\Longrightarrow \quad 4l < 4k + 3 \\ &\Longrightarrow \quad l < k + \frac{3}{4} \\ &\Longrightarrow \quad l < k + \frac{1}{4} \\ &\Longrightarrow \quad \frac{1}{4} < \frac{k+\frac{1}{2}}{n}. \end{aligned}$$

To see that $(iii) \Longrightarrow n_+ > n_-$, notice that there will be a k such that $1/4 \not< k/n$ and $1/4 < (k+1)/n$ so this k makes no contribution to n_- but it does contribute to n_+ since, on account of (iii), $1/4 < (k+1/2)/n$. Finally, since $(k+1/2)/n < (k+1)/n$ then

$$(iv) \quad \frac{k+1}{n} \leq \frac{1}{4} \Longrightarrow \frac{k+\frac{1}{2}}{n} < \frac{1}{4},$$

and it follows that $n_+ = n_- + 1$. To see this we note that if k is such that $k/n \leq 1/4$ and $(k+1)/n \leq 1/4$ then $(k+1/2)/n \leq 1/4$ and so such a k makes no contribution to either n_- or n_+.

Hence, the deficiency indices of $\widehat{T}_{n,o}$ for $n = 4l+1$, where $l = 0, 1, 2, ...$, are $(n_- + 1, n_-)$, so there are no self-adjoint extensions (appendix A). Similarly we can show this for $n = 4l + 3$. In other words, all positive integer powers of the half-line momentum can be identified with observables in our generalised theory but only the even powers can be identified with orthodox observables.

3.4 Quantisation in Generalised Coordinates

So far we have examined some of the difficulties in quantising very simple classical observables at a rigorous level. We have seen, for example, that naively squaring the half-line momentum $\widehat{P}_+$ does not yield a maximal symmetric operator and so the Hamiltonian for a free particle on $\boldsymbol{R}^+$ cannot be identified with the operator $(1/2m)\widehat{P}_+^2$. In this section we shall encounter complications at a formal level. Problems associated with the quantisation of the free particle Hamiltonian in more elaborate coordinate systems are discussed and some inadequacies of current approaches to the problem are highlighted. Since we are to give only a formal treatment, the operator theoretic notions of symmetry, self-adjointness, etc. will not be distinguished and we shall use the term Hermitian to describe an operator which is formally symmetric.

3.4.1 The Hamiltonian for a Single Free Particle in Orthogonal Curvilinear Coordinates

Let R_k denote the range of generalised coordinate q_k and let (g_{kl}) be the appropriate metric tensor with determinant $g \neq 0$.

As we will be dealing only with orthogonal coordinates then [85, p 452]

$$g_{kl} = 0, \qquad k \neq l$$

and we define $\mathcal{G}_k \equiv g_{kk}$, so that g is given by the product $\Pi_k \mathcal{G}_k$. The inverse of (g_{kl}), denoted (g^{kl}), is then defined by

$$g^{kl} = 0, \qquad k \neq l,$$
$$g^{kk} = \frac{1}{\mathcal{G}_k} \equiv \mathcal{G}^k$$

with determinant $1/g$.

The Hamiltonian in generalised coordinates (q_k) is taken to be

$$\begin{aligned} \widehat{H} &= -\frac{\hbar^2}{2m}\nabla^2 \\ &= -\frac{\hbar^2}{2m}\sum_k \frac{1}{\sqrt{g}}\frac{\partial}{\partial q_k}\sqrt{g}\mathcal{G}^k\frac{\partial}{\partial q_k} \end{aligned} \tag{3.6}$$

([86, p 238], [87]) which is Hermitian in the Hilbert space

$$\mathcal{H} = L^2(R_1 \times R_2 \times R_3, \sqrt{g}dq_1dq_2dq_3).$$

Note that $\widehat{H}$ can be expressed thus:

$$\widehat{H} = \frac{1}{2m}\sum_k \frac{1}{g^{\frac{1}{4}}}\widehat{P}_k\sqrt{g}\mathcal{G}^k\widehat{P}_k\frac{1}{g^{\frac{1}{4}}}, \tag{3.7}$$

where $\widehat{P}_k$ is the generalised momentum corresponding to coordinate q_k, which is defined by

$$\widehat{P}_k = -i\hbar\frac{1}{g^{\frac{1}{4}}}\frac{\partial}{\partial q_k}g^{\frac{1}{4}}$$

[87, 88, 89], where $\widehat{P}_k$ is also Hermitian in $\mathcal{H}$.

We can now unambiguously recover the classical Hamiltonian by replacing $\widehat{P}_k$ with P_k, i.e.

$$\widehat{P}_k \longrightarrow P_k \Longrightarrow \widehat{H} \longrightarrow H = \frac{1}{2m}\sum_k \mathcal{G}^k P_k^2.$$

Without knowledge of (3.7), the reverse process is far from trivial [86, pp 237–240], [87, 88, 89, 90, 91, 92]. Simply substituting $\widehat{P}_k$ for P_k in the classical Hamiltonian generally would not yield $\widehat{H}$ as given by (3.6). The source of the problem is that the classical variables appearing in H commute whereas their quantum counterparts do not. Clearly if we wish to obtain (3.6) by a direct substitution of P_k by $\widehat{P}_k$ in the classical Hamiltonian we should use the expression

$$H = \frac{1}{2m}\sum_k \frac{1}{g^{\frac{1}{4}}}P_k\sqrt{g}\mathcal{G}^k P_k\frac{1}{g^{\frac{1}{4}}}. \tag{3.8}$$

Not content with the somewhat cumbersome expression (3.7) and the contrived form of (3.8), Gruber [87] has proposed an alternative scheme for quantising the classical Hamiltonian in generalised coordinates, which we outline next.

In [90], it was realised that $\widehat{P}_k$ is the Hermitian part of the operator $\widehat{p}_k$, which is defined in $\mathcal{H}$ by

$$\widehat{p}_k \equiv -i\hbar\frac{\partial}{\partial q_k},$$

i.e.

$$\widehat{P}_k = \frac{1}{2}\left(\widehat{p}_k + \widehat{p}_k^\dagger\right),$$

where $\widehat{p}_k^\dagger$ is given by[2]

$$\widehat{p}_k^\dagger = -i\hbar\frac{1}{g^2}\frac{\partial}{\partial q_k}g^2.$$

In [87] it is considered to be more accurate to write H as

$$H = \frac{1}{2m}\sum_k P_k^* \mathcal{G}^k P_k, \tag{3.9}$$

even though the classical momenta are assumed to be real variables. In view of (3.9) it is then proposed that the quantised Hamiltonian be given as

$$\widehat{H} = \frac{1}{2m}\sum_k \widehat{p}_k^\dagger \mathcal{G}^k \widehat{p}_k, \tag{3.10}$$

which does indeed coincide with (3.6). However, this scheme does not tell us how to incorporate the momentum $\widehat{P}_k$ into the quantum Hamiltonian, but instead we must use the non-Hermitian operator $\widehat{p}_k$ and its adjoint. It is well known that a general operator is not uniquely determined by its Hermitian part only. This is analogous to a general complex number not being uniquely determined by its real part only. Clearly, expression (3.9) is no less contrived than the expression (3.8). Furthermore, Gruber's classical Hamiltonian, as given by (3.9), is a function of the classical momentum variables P_k. This is at odds with the fact that his quantised Hamiltonian, as given by (3.10), is not a function of the quantum momentum operators $\widehat{P}_k$.

We shall take as our 'natural form' of H the expression

$$H = \frac{1}{2m}\sum_k \mathcal{G}^k P_k^2. \tag{3.11}$$

Of course, this is no more natural than the expression

$$H = \frac{1}{2m}\sum_k P_k^2 \mathcal{G}^k$$

[2]Note that our g corresponds to g^2 in [87, 90].

and it turns out that for the coordinate systems usually treated [87, 89, 90, 91], a direct substitution of $\widehat{P}_k$ for P_k into either expression yields the same operator. However, this is generally not the case for coordinate systems where $\mathcal{G}^k$ depends on q_k as in, for example, parabolic cylindrical coordinates (see later).

If we make the substitution $\widehat{P}_k$ for P_k in (3.11) we get

$$\widehat{H}_c \equiv \frac{1}{2m}\sum_k \mathcal{G}^k \widehat{P}_k^2 = -\frac{\hbar^2}{2m}\sum_k \mathcal{G}^k \frac{1}{g^{\frac{1}{4}}}\frac{\partial^2}{\partial q_k^2} g^{\frac{1}{4}}$$

$$= -\frac{\hbar^2}{2m}\sum_k \left\{ \frac{1}{4g}\mathcal{G}^k \frac{\partial^2 g}{\partial q_k^2} - \frac{3}{16g^2}\mathcal{G}^k \left(\frac{\partial g}{\partial q_k}\right)^2 + \frac{1}{2g}\mathcal{G}^k \frac{\partial g}{\partial q_k}\frac{\partial}{\partial q_k} + \mathcal{G}^k \frac{\partial^2}{\partial q_k^2} \right\}.$$

Expanding out $\widehat{H} = -(\hbar^2/2m)\nabla^2$ yields

$$\widehat{H} = -\frac{\hbar^2}{2m}\sum_k \left\{ \frac{1}{2g}\mathcal{G}^k \frac{\partial g}{\partial q_k}\frac{\partial}{\partial q_k} + \frac{\partial \mathcal{G}^k}{\partial q_k}\frac{\partial}{\partial q_k} + \mathcal{G}^k \frac{\partial^2}{\partial q_k^2} \right\}.$$

So

$$\widehat{H} = \widehat{H}_c + \widehat{H}' \tag{3.12}$$

where

$$\widehat{H}' = -\frac{\hbar^2}{2m}\sum_k \left\{ \frac{\partial \mathcal{G}^k}{\partial q_k}\frac{\partial}{\partial q_k} + \frac{3}{16g^2}\mathcal{G}^k \left(\frac{\partial g}{\partial q_k}\right)^2 - \frac{1}{4g}\mathcal{G}^k \frac{\partial^2 g}{\partial q_k^2} \right\}. \tag{3.13}$$

Recently, a correspondence rule has been proposed by Zhan [89] which is applicable to orthogonal curvilinear coordinate systems. It has the form

$$F(P_k, q_k) \longrightarrow \widehat{F}(\widehat{P}_k, \widehat{q}_k) + D(\widehat{q}_k) \tag{3.14}$$

where F is the classical observable and $\widehat{F}$ is obtained by substituting $\widehat{P}_k$ and $\widehat{q}_k$ for P_k and q_k in F. If F is the classical free particle Hamiltonian then $\widehat{F}$ coincides with $\widehat{H}_c$ above. It is clear from (3.12) and (3.13), that (3.14) does not apply to all orthogonal curvilinear coordinate systems. It is only when $\mathcal{G}^k$ is independent of q_k, can the function D be associated with $\widehat{H}'$ since we then have

$$\widehat{H}' = -\frac{\hbar^2}{2m}\sum_k \left\{ \frac{3}{16g^2}\mathcal{G}^k \left(\frac{\partial g}{\partial q_k}\right)^2 - \frac{1}{4g}\mathcal{G}^k \frac{\partial^2 g}{\partial q_k^2} \right\} \tag{3.15}$$

which is a function of the coordinates $\{q_k\}$ alone. This is true in particular for circular and spherical polar coordinates.

2-D Circular Polars (r, φ)

$$\mathcal{G}^1 = 1, \quad \mathcal{G}^2 = \frac{1}{r^2}, \quad g = r^2,$$

$$H = \frac{1}{2m}\left(P_r^2 + \frac{1}{r^2}P_\varphi^2\right) \Longrightarrow \widehat{H}_c = \frac{1}{2m}\left(\widehat{P}_r^2 + \frac{1}{r^2}\widehat{P}_\varphi^2\right),$$

where

$$\widehat{P}_r = -i\hbar\frac{1}{\sqrt{r}}\frac{\partial}{\partial r}\sqrt{r} = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{2r}\right)$$

and

$$\widehat{P}_\varphi = -i\hbar\frac{\partial}{\partial\varphi}.$$

Substituting the following into (3.15):

$$\frac{\partial g}{\partial r} = 2r, \qquad \frac{\partial^2 g}{\partial r^2} = 2,$$

$$\frac{\partial g}{\partial\varphi} = \frac{\partial^2 g}{\partial\varphi^2} = 0,$$

we get

$$\widehat{H}' = -\frac{\hbar^2}{8mr^2},$$

as of course does Zhan.

3-D Spherical Polars (r, θ, φ)

$$\mathcal{G}^1 = 1, \quad \mathcal{G}^2 = \frac{1}{r^2}, \quad \mathcal{G}^3 = \frac{1}{r^2\sin^2\theta}, \quad g = r^4\sin^2\theta,$$

$$H = \frac{1}{2m}\left(P_r^2 + \frac{1}{r^2}P_\theta^2 + \frac{1}{r^2\sin^2\theta}P_\varphi^2\right) \Longrightarrow \widehat{H}_c = \frac{1}{2m}\left(\widehat{P}_r^2 + \frac{1}{r^2}\widehat{P}_\theta^2 + \frac{1}{r^2\sin^2\theta}\widehat{P}_\varphi^2\right),$$

where

$$\widehat{P}_r = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}r = -\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right),$$

$$\widehat{P}_\theta = -i\hbar\frac{1}{\sqrt{\sin\theta}}\frac{\partial}{\partial\theta}\sqrt{\sin\theta} = -i\hbar\left(\frac{\partial}{\partial\theta} + \frac{\cos\theta}{2\sin\theta}\right),$$

$$\widehat{P}_\varphi = -i\hbar\frac{\partial}{\partial\varphi}.$$

Into (3.15) we substitute the following:

$$\frac{\partial g}{\partial r} = 4r^3\sin^2\theta, \qquad \frac{\partial^2 g}{\partial r^2} = 12r^2\sin^2\theta,$$

$$\frac{\partial g}{\partial \theta} = 2r^4 \sin\theta \cos\theta, \quad \frac{\partial^2 g}{\partial \theta^2} = 2r^4 \left(\cos^2\theta - \sin^2\theta\right),$$
$$\frac{\partial g}{\partial \varphi} = \frac{\partial^2 g}{\partial \varphi^2} = 0$$

and we get

$$\widehat{H}' = -\frac{\hbar^2}{8mr^2}\left(\frac{1+\sin^2\theta}{\sin^2\theta}\right),$$

which again agrees with Zhan.

The next example is an instance where Zhan's correspondence rule does not apply.

Parabolic Cylindrical Coordinates (u, v, z)

(See [84, pp 145–146] and [85, pp 431,434,452].)

$$\mathcal{G}^1 = \mathcal{G}^2 = \frac{1}{u^2+v^2}, \quad \mathcal{G}^3 = 1, \quad g = (u^2+v^2)^2,$$

$$H = \frac{1}{2m}\left(\frac{1}{u^2+v^2}P_u^2 + \frac{1}{u^2+v^2}P_v^2 + P_z^2\right) \Longrightarrow \widehat{H}_c = \frac{1}{2m}\left(\frac{1}{u^2+v^2}\widehat{P}_u^2 + \frac{1}{u^2+v^2}\widehat{P}_v^2 + \widehat{P}_z^2\right),$$

where

$$\widehat{P}_u = -i\hbar\frac{1}{(u^2+v^2)^{\frac{1}{2}}}\frac{\partial}{\partial u}(u^2+v^2)^{\frac{1}{2}} = -i\hbar\left(\frac{\partial}{\partial u} + \frac{u}{u^2+v^2}\right),$$
$$\widehat{P}_v = -i\hbar\left(\frac{\partial}{\partial v} + \frac{v}{u^2+v^2}\right),$$
$$\widehat{P}_z = -i\hbar\frac{\partial}{\partial z}.$$

If we substitute into (3.13) the following:

$$\frac{\partial g}{\partial u} = 4u(u^2+v^2), \quad \frac{\partial^2 g}{\partial u^2} = 4(3u^2+v^2),$$
$$\frac{\partial g}{\partial v} = 4v(u^2+v^2), \quad \frac{\partial^2 g}{\partial v^2} = 4(3v^2+u^2),$$
$$\frac{\partial g}{\partial z} = \frac{\partial^2 g}{\partial z^2} = 0, \quad \frac{\partial \mathcal{G}^1}{\partial u} = -\frac{2u}{(u^2+v^2)^2}, \quad \frac{\partial \mathcal{G}^2}{\partial v} = -\frac{2v}{(u^2+v^2)^2}, \quad \frac{\partial \mathcal{G}^3}{\partial z} = 0,$$

we get

$$\widehat{H}' = \frac{\hbar^2}{2m(u^2+v^2)^2}\left\{1 + 2\left(u\frac{\partial}{\partial u} + v\frac{\partial}{\partial v}\right)\right\},$$

which cannot be expressed as a function of u, v and z alone. Indeed, since

$$\frac{\partial}{\partial u} = \frac{i}{\hbar}\widehat{P}_u - \frac{u}{u^2+v^2} \text{ and } \frac{\partial}{\partial v} = \frac{i}{\hbar}\widehat{P}_v - \frac{v}{u^2+v^2},$$

then we have

$$\widehat{H}' = \frac{\hbar^2}{2m(u^2+v^2)^2}\left\{\frac{2i}{\hbar}(u\widehat{P}_u + v\widehat{P}_v) - 1\right\}.$$

3.5 Isometric Semigroups and Maximal Symmetric Operators

The correspondence between self-adjoint operators and strongly continuous groups of unitary operators can be generalised to a correspondence between maximal symmetric operators and strongly continuous semigroups of isometric operators. This opens up the possibility of describing non-unitary time evolution by allowing non-self-adjoint maximal symmetric Hamiltonians.

The objective of this section is to develop these ideas and apply them to the quantisation of classical Hamiltonians which do not permit global (full time) solutions to their associated equations of motion.

The main references for this section are [61, §§ 141–142] and [94, ch VIII: § 1].

Definition 15 *A family of bounded linear operators $\{T_t : t \geq 0\}$ on a Hilbert space $\mathcal{H}$, for which*

(i) $T_o = \widehat{I}$

(ii) $T_s T_t = T_{s+t} \qquad s, t \geq 0$

(iii) $\lim_{\delta t \to o} \|(T_{t+\delta t} - T_t)\phi\| = 0 \qquad \forall \phi \in \mathcal{H} \quad (t \geq 0)$

is called a strongly continuous (one-parameter) semigroup.

Definition 16 *A strongly continuous semigroup of bounded linear operators $\{T_t : t \geq 0\}$ on a Hilbert space $\mathcal{H}$ is called an isometric semigroup if $\|T_t\phi\| = \|\phi\|$ for all $\phi \in \mathcal{H}$.*

Note that if $\{T_t : t \geq 0\}$ is an isometric semigroup then $\|T_t\| = 1$, so an isometric semigroup is a special instance of a contraction semigroup [50, p 235]. While contraction semigroups are generally dissipative, i.e.

$$\frac{d}{dt}\langle T_t\phi \mid T_t\phi\rangle \leq 0 \qquad \forall \phi \in \mathcal{H},$$

for those which are isometric semigroups we have

$$\frac{d}{dt}\langle T_t\phi \mid T_t\phi\rangle = \frac{d}{dt}\langle \phi \mid \phi\rangle = 0 \qquad \forall \phi \in \mathcal{H}.$$

Also, as T_t is bounded then it has an adjoint $T_t^\dagger$ defined on $\mathcal{H}$. Furthermore

$$\begin{aligned}\langle \psi \mid T_t^\dagger T_t\phi\rangle &= \langle T_t\psi \mid T_t\phi\rangle \\ &= \langle \psi \mid \phi\rangle \qquad \forall \psi, \phi \in \mathcal{H},\end{aligned}$$

so

$$T_t^\dagger T_t = \widehat{I}.$$

In other words T_t possesses the left hand inverse $T_t^\dagger$. However, we generally do not have

$$T_t T_t^\dagger = \widehat{I},$$

though we do have

$$(T_t T_t^\dagger)^2 = T_t(T_t^\dagger T_t)T_t^\dagger = T_t T_t^\dagger,$$

i.e. $T_t T_t^\dagger$ is a projector. This implies

$$\langle T_t^\dagger\phi \mid T_t^\dagger\phi\rangle \leq 1 \qquad \forall \phi \in \mathcal{H}.$$

We now list some general properties of isometric semigroups which may be easily verified (see for example [93]):

(i) For any positive s, t,

$$T_s^\dagger T_t^\dagger = T_{s+t}^\dagger.$$

(ii) If $t \geq s \geq 0$ then

$$T_s^\dagger T_t = T_{t-s}.$$

(iii) If $R(T_t)$ denotes the range of T_t and $P\left(R(T_t)\right)$ is the projection onto $R(T_t)$ then

$$P\left(R(T_t)\right) = T_t T_t^\dagger.$$

(iv) If $t < s$ then

$$R(T_t) \supset R(T_s).$$

Since $T_o^\dagger = \widehat{I}$ then it follows from (i) that $\{T_t^\dagger : t \geq 0\}$ also forms a semigroup and properties (iii) and (iv) show it to be dissipative.

Definition 17 *Let $\{T_t : t \geq 0\}$ be a strongly continuous semigroup on a Hilbert space $\mathcal{H}$ and define the linear operator $\widehat{Z}_t$ by*

$$\widehat{Z}_t\phi = \frac{1}{t}(T_t - \widehat{I})\phi, \qquad \phi \in \mathcal{H}.$$

Let $\mathcal{D}(\widehat{Z})$ be the set of all $\phi \in \mathcal{H}$ for which $\lim_{t\downarrow o} \widehat{Z}_t\phi$ exists and define $\widehat{Z}$ with domain $\mathcal{D}(\widehat{Z})$ by

$$\widehat{Z}\phi = \lim_{t\downarrow o} \widehat{Z}_t\phi \qquad \phi \in \mathcal{D}(\widehat{Z}).$$

The operator $\widehat{Z}$ with domain $\mathcal{D}(\widehat{Z})$ is called the infinitesimal generator of the semigroup $\{T_t : t \geq 0\}$.

Some elementary properties of the infinitesimal generator are given by the following ([61, p 398],[94, p 619])

Theorem 14 *For $\{T_t : t \geq 0\}$ and $\widehat{Z}$ as above, we have:*

(i) *$\mathcal{D}(\widehat{Z})$ is dense in $\mathcal{H}$.*

(ii) *$\widehat{Z}$ is a closed linear operator.*

(iii) *If $\phi \in \mathcal{D}(\widehat{Z})$ then $T_t\phi \in \mathcal{D}(\widehat{Z})$ and*

$$\frac{d}{dt}T_t\phi = \widehat{Z}T_t\phi = T_t\widehat{Z}\phi, \qquad t \in \boldsymbol{R}^+.$$

As is well known, every strongly continuous group of unitary operators is related to a self-adjoint operator through the infinitesimal generator of the group. The generalised result, applicable to strongly continuous semigroups of isometric operators, is given by the following [55, p 1258] (see also [61, p 396], [95, p 153]):[3]

[3]Though this theorem caters only for maximal symmetric operators which have $n_+ = 0$, it can be extended to apply generally. Recall from appendix A that if $\widehat{A}$ is maximal symmetric with deficiency indices (n_+, n_-) then $-\widehat{A}$ is maximal symmetric with deficiency indices (n_-, n_+). So, if $n_- = 0$ then $-i\widehat{A}$ is the infinitesimal generator of an isometric semigroup. Alternatively, we can redefine a semigroup in terms of a negative parameter, i.e. $\{T_t : t \leq 0\}$, and proceed as before except that here, the infinitesimal generators would be of the form $i\widehat{A}$ where $\widehat{A}$ is maximal symmetric with $n_- = 0$.

Theorem 15 *If* $\{T_t : t \geq 0\}$ *is a strongly continuous isometric semigroup then its infinitesimal generator is of the form* $i\widehat{A}$ *where* $\widehat{A}$ *is maximal symmetric with deficiency indices* (n_+, n_-) *such that* $n_+ = 0$. *Conversely if* $\widehat{A}$ *is maximal symmetric with* $n_+ = 0$ *then* $i\widehat{A}$ *is the infinitesimal generator of a one parameter strongly continuous isometric semigroup.*

As an illustration we shall consider the example of the translation semigroup of isometries $\{T_t : t \geq 0\}$ on $L^2(\mathbb{R}^+)$ defined by

$$(T_t\phi)(x) = \begin{cases} \phi(x-t) & \forall x \geq t \\ 0 & \forall x < t \end{cases}$$

cf. [61, p 396].

We shall investigate the convergence or otherwise of the sequence $(1/t)\left(T_t - \widehat{I}\right)\phi(x)$ as $t \downarrow 0$. For $x \geq t$, $\{T_t : t \geq 0\}$ behaves like the translation group generated by the usual momentum operator $\widehat{P}$ in $L^2(\mathbb{R})$. So, provided $x > 0$ and $\phi \in AC(\mathbb{R}^+)$, the limit exists. For $x = 0$ the limit becomes $\lim_{t\downarrow o}(-\phi(0)/t)$, which exists only if $\phi(0) = 0$. So, on $AC(\mathbb{R}^+)$ such that $\phi(0) = 0$, we have

$$\lim_{t\downarrow o} \frac{T_t\phi - \phi}{t} = -\frac{d\phi}{dx},$$

i.e. the infinitesimal generator is $\widehat{Z}$ defined on

$$\mathcal{D}(\widehat{Z}) = \left\{\phi \in L^2(\mathbb{R}^+) : \phi \in AC(\mathbb{R}^+), \phi' \in L^2(\mathbb{R}^+), \phi(0) = 0\right\}$$

by

$$\widehat{Z}\phi = -\frac{d\phi}{dx}.$$

Now $\widehat{Z} = i\widehat{A}$ where $\widehat{A} = (-1/\hbar)\widehat{P}_+$ and $\widehat{A}$ is maximal symmetric with deficiency indices $(0, 1)$ (appendix A).

The following theorem is from [55, p 1258].

Theorem 16 *If* $\{T_t : t \geq 0\}$ *is a strongly continuous semigroup of operators on a Hilbert space* $\mathcal{H}$ *with infinitesimal generator* $\widehat{Z}$ *then* $\{T_t^\dagger : t \geq 0\}$ *is a strongly continuous semigroup on* $\mathcal{H}$ *with infinitesimal generator* $\widehat{Z}^\dagger$.

For an isometric semigroup $\{T_t : t \geq 0\}$ whose generator is $i\widehat{A}$, $\widehat{A}$ being maximal symmetric, the infinitesimal generator for $\{T_t^\dagger : t \geq 0\}$ will be $(i\widehat{A})^\dagger = -i\widehat{A}^\dagger$. As an illustration we shall examine the semigroup $\{T_t^\dagger : t \geq 0\}$ where $\{T_t : t \geq 0\}$ is the translation semigroup defined earlier. For arbitrary $\psi, \phi \in L^2(\boldsymbol{R}^+)$ we have

$$\begin{aligned}\langle \psi \mid T_t\phi \rangle &= \int_t^\infty \psi^*(x)\phi(x-t)dx \qquad \forall t \geq 0 \\ &= \int_0^\infty \psi^*(x'+t)\phi(x')dx', \qquad x' = x - t,\end{aligned}$$

so that

$$\left(T_t^\dagger \phi\right)(x) = \phi(x+t) \qquad \forall t \geq 0.$$

Let $\widehat{Z}'$ be the infinitesimal generator of $\{T_t^\dagger : t \geq 0\}$. We know from theorem 16 that $\widehat{Z}' = \widehat{Z}^\dagger$. This is easily verified:

$$\lim_{t \downarrow o} \frac{1}{t}(T_t^\dagger - \widehat{I})\phi = \lim_{t \downarrow o} \frac{\phi(x+t) - \phi(x)}{t}$$

which exists without imposing any restriction on ϕ at the origin and so $\widehat{Z}' = d/dx$ on $AC(\mathbb{R}^+)$, i.e. $\widehat{Z}' = (i/\hbar)\widehat{P}_+^\dagger = \widehat{Z}^\dagger$.

Though $\{T_t^\dagger : t \geq 0\}$ is a strongly continuous semigroup, it is not an isometric semigroup since

$$\begin{aligned}\langle T_t^\dagger \phi \mid T_t^\dagger \phi \rangle &= \int_0^\infty \phi^*(x+t)\phi(x+t)dx \\ &= \int_t^\infty |\phi(x)|^2 dx \leq \int_0^\infty |\phi(x)|^2 dx,\end{aligned}$$

where the equality holds only for those ϕ with null support in $(0, t)$. Also, since

$$\langle T_t^\dagger \phi \mid T_t^\dagger \phi \rangle = -\int_\infty^t |\phi(x)|^2 dx,$$

then almost everywhere we have

$$\frac{d}{dt}\langle T_t^\dagger \phi \mid T_t^\dagger \phi \rangle = -|\phi(t)|^2,$$

which shows the dissipative nature of $\{T_t^\dagger : t \geq 0\}$; see [22, pp 555–556] for pictures. Furthermore, by monotone convergence [63, p 95]:

$$\begin{aligned}\lim_{t \to \infty} \langle T_t^\dagger \phi \mid T_t^\dagger \phi \rangle &= \lim_{t \to \infty} \int_0^\infty \chi_{(t,\infty)}(x)|\phi(x)|^2 dx \\ &= 0 \qquad \forall \phi \in L^2(\boldsymbol{R}^+),\end{aligned}$$

i.e. $\{T_t^\dagger : t \geq 0\}$ is completely non-unitary [95, p 155].

3.5.1 Temporal Evolution

The 'dynamics axiom' of orthodox quantum mechanics states that the temporal evolution of the state of a system is governed by a strongly continuous unitary group $\{U_t : t \in \mathbb{R}\}$ on an appropriate Hilbert space $\mathcal{H}$. Stone's theorem tells us that the infinitesimal generator of such a group is of the form $i\widehat{H}$ where $\widehat{H}$ is self-adjoint; so Stone's theorem is a special case of theorem 15. The operator $\widehat{H}$ is called the Hamiltonian.

We are to look at the dynamics generated by maximal symmetric, but not necessarily self-adjoint, Hamiltonians. For example assume $\widehat{H} = \widehat{P}_+$. From the above analysis, we can see immediately that $-i\widehat{H}$ generates the dynamics in which a wavepacket travels to the right with constant (unit) velocity. Let $\{T_t : t \geq 0\}$ be the relevant semigroup, i.e. the translation semigroup on $\mathbb{R}^+$, then the left hand inverse semigroup $\{T_t^\dagger : t \geq 0\}$ which, by theorem 16, has as its infinitesimal generator $i\widehat{H}^\dagger$ is seen to have the effect of evolving the wavepacket towards the origin with constant velocity. As $t \to \infty$, $\langle T_t^\dagger \phi \mid T_t^\dagger \phi \rangle \to 0$ and the wavepacket is apparently absorbed into the origin.[4] The physical reason for this is that a particle cannot travel indefinitely to the left with constant velocity and remain in $\mathbb{R}^+$. A similar analysis applies in the case where $\widehat{H}$ is taken to be the radial momentum $\widehat{P}_r$. A free particle cannot remain in a state of constant non-zero radial momentum for all time. This is consistent with the fact that $\widehat{P}_r$ does not possess generalised eigenfunctions (cf. chapter 1).

Completing the Dynamics

It is noticeable that the dynamics generated by $-i\widehat{H}$ with $\widehat{H} = \widehat{P}_+$ can also be regarded as being generated by $-i\widehat{H}_\sim$ with $\widehat{H}_\sim = \widehat{P}$, where $\widehat{P}$ is the usual momentum operator defined in $L^2(\mathbb{R})$, when applied to those $\phi_\sim \in L^2(\mathbb{R})$ with support in $\mathbb{R}^+$ only. For the

[4]This behaviour resembles that associated with 'absorbed states', a notion familiar to scattering theorists [96, p 467]. Since, if $T_t^\dagger \phi$ describes the state of a particle in $\mathbb{R}^+$, then the probability of finding the particle outside any small neighbourhood of $x = 0$ vanishes as $t \to \infty$.

general case we have the following ([61, pp 396,472], [95, p 161])

Theorem 17 *If $\{T_t : t \geq 0\}$ is an isometric semigroup on a Hilbert space $\mathcal{H}$, there is a larger Hilbert space $\mathcal{H}_\sim \supset \mathcal{H}$ on which there exists a unitary group $\{U_t : t \in \mathbb{R}\}$ such that for $t \geq 0$,*

$$T_t\phi = U_t\phi \qquad \forall\phi \in \mathcal{H}.$$

Now suppose $\{T_t : t \geq 0\}$ is an isometric semigroup on a Hilbert space $\mathcal{H}$ with infinitesimal generator $i\widehat{A}$, $\widehat{A}$ maximal symmetric. By theorem 17 we know that there exists a unitary group $\{U_t : t \in \mathbb{R}\}$ on a Hilbert space $\mathcal{H}_\sim \supset \mathcal{H}$ such that $T_t = U_t$, $t \geq 0$. If the infinitesimal generator of $\{U_t : t \in \mathbb{R}\}$ is $i\widehat{A}_\sim$ then, by Stone's theorem, $\widehat{A}_\sim$ is self-adjoint. Also, $i\widehat{A}_\sim$ is the infinitesimal generator of the semigroup of unitary operators $\{U_t : t \geq 0\}$ [94, pp 619,627–628].[5] Now

$$\mathcal{D}(\widehat{A}_\sim) = \left\{\psi_\sim \in \mathcal{H}_\sim : \lim_{t\downarrow o} \frac{1}{t}(U_t - \widehat{I})\psi_\sim \text{ exists}\right\},$$

and

$$\begin{aligned}\mathcal{D}(\widehat{A}) &= \left\{\phi \in \mathcal{H} : \lim_{t\downarrow o} \frac{1}{t}(T_t - \widehat{I})\phi \text{ exists}\right\} \\ &= \left\{\phi \in \mathcal{H} : \lim_{t\downarrow o} \frac{1}{t}(U_t - \widehat{I})\phi \text{ exists}\right\}.\end{aligned}$$

Hence $\mathcal{D}(\widehat{A}) = \mathcal{D}(\widehat{A}_\sim) \cap \mathcal{H}$. Now for each $\phi \in \mathcal{D}(\widehat{A})$ we have

$$\begin{aligned}i\widehat{A}\phi &= \lim_{t\downarrow o} \frac{1}{t}(T_t - \widehat{I})\phi \\ &= \lim_{t\downarrow o} \frac{1}{t}(U_t - \widehat{I})\phi = i\widehat{A}_\sim\phi,\end{aligned}$$

so $\widehat{A}_\sim$ is a generalised self-adjoint extension of $\widehat{A}$. Let $\widehat{P}_\sim$ be the projector on $\mathcal{H}_\sim$ of range $\mathcal{H}$. Since for arbitrary $\phi_\sim \in \mathcal{H}_\sim$ we have [61, pp 383–385]

$$U_t\phi_\sim = \int_{-\infty}^{\infty} e^{i\lambda t} d_\lambda \widehat{E}(\widehat{A}_\sim;\lambda)\phi_\sim$$

[5] Note that an arbitrary semigroup of unitary operators $\{U_t : t \geq 0\}$ can be extended to a unitary group simply by defining U_{-t} to be U_t^{-1}.

then for $\phi \in \mathcal{H}$ we have, on account of $\widehat{P}_\sim$ being continuous,

$$\begin{aligned} \widehat{P}_\sim U_t\phi &= \int_{-\infty}^{\infty} e^{i\lambda t} d_\lambda \widehat{P}_\sim \widehat{E}(\widehat{A}_\sim;\lambda)\phi \\ &= \int_{-\infty}^{\infty} e^{i\lambda t} d_\lambda \widehat{F}(\widehat{A};\lambda)\phi, \end{aligned}$$

where $\widehat{F}(\widehat{A};\lambda)$ is the (generalised) spectral function of $\widehat{A}$. We have thus proved the following

Theorem 18 *Every one-parameter isometric semigroup $\{T_t : t \geq 0\}$ admits the representation*

$$T_t = \int_{-\infty}^{\infty} e^{i\lambda t} d_\lambda \widehat{F}(\widehat{A};\lambda)$$

where strong convergence is understood and $\widehat{F}(\widehat{A};\lambda)$ is the generalised spectral function of a maximal symmetric symmetric operator $\widehat{A}$ such that $i\widehat{A}$ is the infinitesimal generator of $\{T_t : t \geq 0\}$.

As an illustration we take: $\mathcal{H} = L^2(\mathbb{R}^+)$, $\mathcal{H}_\sim = L^2(\mathbb{R})$, $\widehat{A} = -(1/\hbar)\widehat{P}_+$, $\widehat{A}_\sim = -(1/\hbar)\widehat{P}$. We know that $-\widehat{P}$ is a generalised self-adjoint extension of $-\widehat{P}_+$ [11, p 139] and so for each $\phi \in \mathcal{H}$,

$$\widehat{F}(-\widehat{P}_+;\lambda)\phi = \widehat{E}(\widehat{X};\mathbb{R}^+)\widehat{E}(-\widehat{P};\lambda)\phi.$$

For arbitrary $\phi \in \mathcal{H}_\sim$ we have

$$\left(\widehat{E}(\widehat{P};\lambda)\phi\right)(x) = \frac{1}{2\pi}\int_{-\infty}^{\lambda} d\lambda' \int_{-\infty}^{\infty} dx' e^{i\lambda'(x-x')}\phi(x').$$

Now

$$\widehat{E}(-\widehat{P};\lambda) = \widehat{E}\left(-\widehat{P};(-\infty,\lambda]\right) = \widehat{E}\left(\widehat{P};[-\lambda,\infty)\right),$$

so

$$\begin{aligned} \left(\widehat{E}(-\widehat{P};\lambda)\phi\right)(x) &= \frac{1}{2\pi}\int_{-\lambda}^{\infty} d\lambda' \int_{-\infty}^{\infty} dx' e^{i\lambda'(x-x')}\phi(x') \\ &= \frac{1}{2\pi}\int_{-\infty}^{\lambda} d\lambda' \int_{-\infty}^{\infty} dx' e^{-i\lambda'(x-x')}\phi(x') \end{aligned}$$

and it follows that for arbitrary $\phi \in \mathcal{H}$, we have

$$\left(\widehat{F}(\widehat{A};\lambda)\phi\right)(x) = \frac{1}{2\pi}\int_{-\lambda}^{\infty} d\lambda' \int_{0}^{\infty} dx' e^{i\lambda'(x-x')}\phi(x').$$

By theorem 18,

$$T_t\phi = \int_{-\infty}^{\infty} e^{i\lambda t} d_\lambda \widehat{F}(\widehat{A};\lambda)\phi = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\lambda t} d_\lambda \int_{-\lambda}^{\infty} d\lambda' \int_0^{\infty} dx' e^{i\lambda'(x-x')}\phi(x')$$
$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda e^{i\lambda t} \int_0^{\infty} dx' e^{-i\lambda(x-x')}\phi(x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda \int_0^{\infty} dx' e^{-i\lambda(x-t-x')}\phi(x').$$

The range of integration for the second integral can be extended to the whole of $\mathbb{R}$ by defining $\phi(x) = 0$ for $x < 0$. So now for $x \geq 0$

$$\begin{aligned}(T_t\phi)(x) &= \left(\lim_{\lambda\to\infty} \widehat{E}\left((-1/\hbar)\widehat{P};\lambda\right)\phi\right)(x-t) \\ &= \phi(x-t),\end{aligned}$$

which is zero if $x - t < 0$. Clearly, $\{T_t : t \geq 0\}$ is the translation semigroup given earlier.

Recently, Zhu and Klauder [97, 98] have demonstrated the link between a non-global solution in classical mechanics and the non-self-adjointness of the quantised Hamiltonian. They view non-self-adjoint Hamiltonians as problematical because they do not give rise to unitary groups, which they regard as the only acceptable quantum mechanical description of dynamics. If, however, we permit semigroups of isometric operators as a description of quantum dynamics then there should be no objection to allowing non-self-adjoint maximal symmetric Hamiltonians, since, for a given such operator $\widehat{H}$, either $-i\widehat{H}$ or $i\widehat{H}$ (but not both) is the infinitesimal generator of an isometric semigroup $\{T_t : t \geq 0\}$ and $i\widehat{H}^\dagger$ (resp. $-i\widehat{H}^\dagger$) is the infinitesimal generator of the left inverse semigroup $\{T_t^\dagger : t \geq 0\}$.

We will now look at some examples of classical Hamiltonians related to those of Zhu and Klauder which correspond to quantum dynamics governed by strongly continuous semigroups of isometric, but not necessarily unitary, operators. In particular we wish to compare the various ways of completing the dynamics quantum mechanically, i.e. extending an isometric semigroup to a unitary group, with the different ways in which the corresponding classical dynamics can be completed.

Consider first the classical Hamiltonian $H(p, x)$ defined on the restricted phase space $\mathbb{R} \times \mathbb{R}^+$, where $\mathbb{R}^+ = [0, \infty)$, by $H = p$. We have

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = 1.$$

A typical solution is $x(t) = t$, and H generates the dynamics in which a particle moves away from the origin in $\mathbb{R}^+$ with constant (unit) velocity. Clearly there is no solution for $t < 0$.

It is a trivial matter to extend H so that there is a solution for all time. We may define $H'(p, x)$ on the phase space $\mathbb{R} \times \mathbb{R}$ by $H' = p$, to obtain $x = t$ for all t.

We wish now to give a quantum mechanical treatment of the same problem. Consider $\widehat{H} = \widehat{P}_+$ defined in $L^2(\mathbb{R}^+)$. We have already seen that $-i\widehat{H}$ generates the dynamics of a particle in $\mathbb{R}^+$ moving away from the origin with constant velocity. We now extend $\widehat{H}$ to $L^2(\mathbb{R})$ in the following manner. Define $\widehat{P}_-$ by

$$\mathcal{D}(\widehat{P}_-) = \left\{\phi \in L^2(\mathbb{R}^-) : \phi \in AC(\mathbb{R}^-), \phi' \in L^2(\mathbb{R}^-), \phi(0) = 0\right\}$$

and

$$\widehat{P}_-\phi = -i\hbar\frac{d\phi}{dx} \qquad \forall\phi \in \mathcal{D}(\widehat{P}_-),$$

where $\mathbb{R}^- = (-\infty, 0]$. The deficiency indices of $\widehat{P}_-$ are $(0, 1)$ [11, p 138], [55, p 1272]. Now $L^2(\mathbb{R}) = L^2(\mathbb{R}^-) \oplus L^2(\mathbb{R}^+)$ and we construct $\widehat{P}_o = \widehat{P}_- \oplus \widehat{P}_+$ on $\mathcal{D}(\widehat{P}_o) = \mathcal{D}(\widehat{P}_-) \oplus \mathcal{D}(\widehat{P}_+)$ where $\widehat{P}_o$ is a closed symmetric operator with deficiency indices $(1, 1)$ and $\widehat{P}_o$ possesses a one parameter family of self-adjoint extensions $\{\widehat{P}_\theta : \theta \in \mathbb{R}\}$ in $L^2(\mathbb{R})$. The self-adjoint extensions of $\widehat{P}_o$ are given by

$$\mathcal{D}(\widehat{P}_\theta) = \left\{\phi \in L^2(\mathbb{R}) : \phi_\pm \in AC(\mathbb{R}^\pm), \phi(0^-) = e^{i\theta}\phi(0^+), \phi' \in L^2(\mathbb{R})\right\}$$

$$\widehat{P}_\theta\phi = -i\hbar\frac{d\phi}{dx} \qquad \forall\phi \in \mathcal{D}(\widehat{P}_\theta).$$

The proof of this is identical to that in appendix E. Note that since $\phi_\pm \in AC(\mathbb{R}^\pm)$ and $\phi(0^-) = \phi(0^+)$ if and only if $\phi \in AC(\mathbb{R})$ [32, p 289] then $\widehat{P}_\theta$, for $\theta = 0$, coincides with the usual momentum operator $\widehat{P}$ in $L^2(\mathbb{R})$. As $\widehat{P}_\theta$ is self-adjoint, $-i\widehat{P}_\theta$ will be the infinitesimal generator of a one parameter semigroup of unitary operators, $\{U_t^\theta : t \geq 0\}$ say, where

$$\left(U_t^\theta\phi\right)(x) = \begin{cases} e^{i\theta}\phi(x - t) & \forall x \in (0, t) \\ \phi(x - t) & \forall x \notin (0, t). \end{cases}$$

The easiest way to see this is to follow the reasoning in [50, pp 142–143] as applied to the 'particle in a box' problem.

So a wavefunction which is translated by the action of U_t^θ picks up a phase factor of $e^{i\theta}$ as it passes through the origin. Clearly the case $\theta = 0$ gives the standard translation semigroup on $\mathbb{R}$ which is generated by the usual momentum operator $\widehat{P}$ in $L^2(\mathbb{R})$.

Physical Significance of the Phase Factor

The system being considered was originally identified with the Hilbert space $\mathcal{H} \equiv L^2(\mathbb{R}^+)$, so modifying any $\phi \in \mathcal{H}$ by an arbitrary phase factor $e^{i\theta}$, i.e. $\phi \longrightarrow e^{i\theta}\phi : \theta \in \mathbb{R}$, has no physical consequence, i.e. produces no observable effect. So, on physical grounds, we expect in our extended system $\mathcal{H}_\sim \equiv L^2(\mathbb{R})$ that wavefunctions are allowed to be modified by an arbitrary phase factor when they are evolved across the origin into $\mathbb{R}^+$, since all such wave functions are physically the same (i.e. represent the same physical state) when restricted to $\mathcal{H}$. From this viewpoint all of the extensions are equally valid and the non-uniqueness is of no physical significance. It would be an entirely different matter of course if the system was originally identified with the Hilbert space $L^2(\mathbb{R})$ instead and we were to start with the family $\{\widehat{P}_\theta : \theta \in \mathbb{R}\}$. Then θ *would* have physical significance and the choice we make for a particular value of θ would depend on some extra physical assumptions. See for example the derivation of Josephson's equation in chapter 1.

For our next example we shall consider the classical Hamiltonian $H(p,x)$ defined on the restricted phase spce $\mathbb{R} \times \mathbb{R}^+$ by $H = -2px^n$ where n is an integer greater than 1. We have

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = -2x^n$$

and typically,

$$x(t) = \sqrt[(n-1)]{\frac{1}{2(n-1)t}}.$$

A solution clearly exists for all $t \geq 0$. For $t < 0$ we have that for n even $x(t) < 0$ and for n odd $x(t)$ becomes complex. So there is no solution for $t < 0$ for any n. We will now attempt to extend H as in the previous example so as to obtain a global solution. We define $H'(p,x)$ on $\boldsymbol{R} \times \mathbb{R}$ by $H' = -2px^n$ to obtain the solution

$$x(t) = (\pm 1)^n \sqrt[(n-1)]{\frac{1}{2(n-1)t}}.$$

So for n even we obtain a global solution, for example $n = 2$, $x(t) = 1/(2t)$ which is valid for all time. For n odd $x(t)$ is still complex for $t < 0$ and we do not have a global solution, for example $n = 3$, $x = \pm\sqrt{1/4t}$. Now for a quantum mechanical treatment. We quantise H thus

$$\widehat{H} = -(\widehat{P}\widehat{X}^n + \widehat{X}^n\widehat{P}) \qquad n > 1.$$

Consider first $\widehat{H}$ defined in $L^2(\mathbb{R}^+)$, call this $\widehat{H}_+$. Now $\widehat{H}_+$ has deficiency indices $(1,0)$ for arbitrary n [55, p 1272], [98].

Next consider $\widehat{H}$ defined in $L^2(\mathbb{R}^-)$, call this $\widehat{H}_-$. If n is even, $\widehat{H}_-$ has deficiency indices $(0,1)$ and if n is odd, $\widehat{H}_-$ has deficiency indices $(1,0)$ (ibid.).

Now construct $\widehat{H} \equiv \widehat{H}_- \oplus \widehat{H}_+$, which is defined in $L^2(\boldsymbol{R})$. For n even $\widehat{H}$ is a closed symmetric operator with deficiency indices $(1,1)$ [42, pp 145,149] and $\widehat{H}$ possesses a one parameter family of self-adjoint extensions $\{\widehat{H}_\theta : \theta \in \mathbb{R}\}$ in $L^2(\mathbb{R})$. So for arbitrary θ, $-i\widehat{H}_\theta$ generates a unitary group on $L^2(\boldsymbol{R})$ which, when restricted to $L^2(\mathbb{R}^+)$, coincides, for $t \geq 0$, with the isometric semigroup generated by $-i\widehat{H}_+$.

For n odd, $\widehat{H}$ is again a closed symmetric operator but this time with deficiency indices $(2,0)$ (ibid.), so $\widehat{H}$ is maximal symmetric in $L^2(\mathbb{R})$ and $-i\widehat{H}$ is the infinitesimal generator of a non-unitary isometric semigroup on $L^2(\mathbb{R})$.

The final example concerns the classical Hamiltonian $H(p,x)$ defined on $\boldsymbol{R} \times \mathbb{R}_o$, where $\mathbb{R}_o = \mathbb{R} - \{0\}$, by

$$H = \frac{x}{|x|}p.$$

We consider H on $\boldsymbol{R} \times \mathbb{R}_o^-$ and on $\mathbb{R} \times \mathbb{R}_o^+$ separately. On $\boldsymbol{R} \times \mathbb{R}_o^-$ we have

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = -1$$

and a typical solution is

$$x(t) = -t.$$

Likewise on $\mathbb{R} \times \mathbb{R}_o^+$ we have

$$x(t) = t.$$

We see that H generates the dynamics of a particle moving away from the origin with constant velocity and there is no solution for $t < 0$. So a system whose dynamics are governed by such a Hamiltonian has no history before $t = 0$; obviously a particle moving away from the origin with constant velocity cannot always have done so.

We now parallel this treatment quantum mechanically by considering the pair of Hamiltonians $\widehat{H}_-$ and $\widehat{H}_+$ defined by

$$\widehat{H}_- = -\widehat{P}_-^o \text{ and } \widehat{H}_+ = \widehat{P}_+^o;$$

where $\widehat{P}_\pm^o$ is essentially the same as $\widehat{P}_\pm$ given earlier except that it is defined in $L^2(\mathbb{R}_o^\pm)$ instead of $L^2(\mathbb{R}^\pm)$. Now the deficiency indices of $\widehat{H}_-$ and $\widehat{H}_+$ are the same, namely $(1, 0)$ and we know from our earlier study of the infinitesimal generator $-i\widehat{P}_+$, that $-i\widehat{P}_+^o$ generates the dynamics in which a wavepacket in $L^2(\mathbb{R}_o^+)$ is evolved to the right with constant velocity. Likewise we can show that $i\widehat{P}_-^o$ generates the dynamics in which a wavepacket in $L^2(\mathbb{R}_o^-)$ is evolved to the left with constant velocity. Next construct $\widehat{H} = \widehat{H}_- \oplus \widehat{H}_+$ defined in $L^2(\mathbb{R})$. From [42, pp 145,149] we have that $\widehat{H}$ is a closed symmetric operator with deficiency indices $(2, 0)$, so $-\widehat{H}$ is maximal symmetric with deficiency indices $(0, 2)$ and $-i\widehat{H}$ is the infinitesimal generator of the dynamics in which the wavefunction is evolved away from the origin with constant velocity. Contrast this with the earlier example that required us to find the maximal symmetric extensions of $\widehat{P}_o \equiv \widehat{P}_- \oplus \widehat{P}_+$ in order to obtain the set of relevant Hamiltonians. Each of these Hamiltonians was self-adjoint and could be identified by a particular boundary condition at the origin. For the example $\widehat{H} \equiv -\widehat{P}_-^o \oplus \widehat{P}_+^o$ being considered here though, $\widehat{H}$ is already maximal symmetric and we do not need to impose any modified boundary condition at the origin. This would be expected since $\widehat{H}$ governs the dynamics in which the wavefunction is dispersed away from the origin. So, if for example the wavefunction has support in only $\mathbb{R}_o^+$ (resp. $\mathbb{R}_o^-$) then it will always have support in only $\mathbb{R}_o^+$ (resp. $\mathbb{R}_o^-$) and we do not have to specify the effect on a wavefunction which is translated through the origin, as we did for the case $\widehat{P}_o$ by choosing a particular self-adjoint extension (value for θ), since this cannot occur.

General Remarks

We have seen that there is no problem in handling the incomplete dynamics associated with non-self-adjoint maximal symmetric Hamiltonians provided we allow a description in terms of isometric semigroups instead of the conventional unitary groups. It is only when one considers the 'generalised Schrödinger equation' does one encounter difficulties, as Cooper discovered nearly fifty years ago [99, 100]: If $\widehat{H}$ is a maximal symmetric operator with domain $\mathcal{D}(\widehat{H})$ then the Schrödinger type equation

$$\widehat{H}\psi(t) = -i\frac{d\psi}{dt} \tag{3.16}$$

with given initial conditions $\psi(0) = \phi \in \mathcal{D}(\widehat{H})$ has a solution for all t if and only if $\widehat{H}$ is self-adjoint. If $\widehat{H}$ has deficiency indices (n_+, n_-) such that $n_+ = 0$ then (3.16) has a solution for all $t > 0$ and if $\widehat{H}$ is such that $n_- = 0$ then (3.16) has a solution for all $t < 0$.

One seemingly unattractive property of maximal symmetric Hamiltonians which are not self-adjoint, with regard to them being energy operators, is the fact that they are not bounded from below. In other words if $\widehat{H}$ is a non-self-adjoint maximal symmetric Hamiltonian then there exists no real number c such that

$$\langle \phi \mid \widehat{H}\phi \rangle \geq c \qquad \forall \phi \in \mathcal{D}(\widehat{H}).$$

This follows from the fact that a semi-bounded symmetric operator has equal deficiency indices [11, p 115] and is therefore self-adjoint or will have self-adjoint extensions.

Orthodox energy observables, i.e. self-adjoint Hamiltonians, are usually deemed unphysical if they are not bounded from below. One place where they do arise however is in the study of unstable systems [101, 102, 103]: Let $\mathcal{H}_u$ denote the Hilbert space of states for an unstable system. It is assumed that the evolution of these states for $t > 0$ is governed by a strongly continuous completely non-unitary contractive semigroup $\{V_t : t \geq 0\}$. Furthermore $\{V_t : t \geq 0\}$ is assumed to be the restriction to $\mathcal{H}_u$ of a strongly continuous unitary semigroup $\{U_t : t \geq 0\}$ on a Hilbert space $\mathcal{H} \supset \mathcal{H}_u$ such that $\mathcal{H} \ominus \mathcal{H}_u$ coincides with the Hilbert space of states for the decay products. If $i\widehat{H}$ is the infinitesimal generator of $\{U_t : t \geq 0\}$, where $\widehat{H}$ is of course self-adjoint, then it turns out that $\sigma(\widehat{H}) = \boldsymbol{R}$ and so $\widehat{H}$ is not bounded from below. The usual conclusion is that this 'semigroup description' of unstable systems cannot be exactly valid. As an approximation however, it has proved to be very successful [42, § 9.6].

In view of the above comments, we should point out that although the non-bounded-from-below property of a non-self-adjoint maximal symmetric operator may discredit it as representing an energy observable, this is no reason to deny it the role of Hamiltonian. The reason for this is that the Hamiltonian of a system need not be an energy observable. A well known example concerns a system which possesses a superselection rule. For such a system it is possible to construct a unitary time evolution which effects transitions between supersectors. The (self-adjoint) Hamiltonian associated with the infinitesimal generator of such a time evolution is not decomposable and therefore is not an observable of the system [64].

Conclusion and Outlook

One mode of introduction for including POV measures as observables is to consider the non-ideal measurement of an orthodox observable, i.e. a self-adjoint operator or PV measure. Each member of the family of probability distribution functions generated by the ORI corresponding to a PV measure is randomised and the resulting modified family, which may be generated by a GRI, is said to describe a non-ideal or approximate observable. This GRI corresponds to a unique POV measure, which, by its construction, is interpreted as an 'unsharp' version of the original PV measure.

Reversing this scenario, we have determined which GRIs can be regarded as observables in the context of ideal measurement and which should be considered as approximate observables measured by means of non-ideal apparatus. The former was found not to be just the set of spectral functions of self-adjoint operators, i.e. the ORIs, as in the orthodox theory, but instead the larger set of spectral functions of maximal symmetric operators, which, in general, are not projector-valued.

A criticism sometimes made of existing generalisations of orthodox quantum mechanics which permit arbitrary POV measures to represent observables, is that there is no corresponding generalisation of the spectral theorem. The theory presented here though *does* admit such a 'generalised spectral theorem'. This takes the form of a one-to-one correspondence between those GRIs which generate maximal families of probability distribution functions and the maximal symmetric operators.

Our generalisation, which requires that an observable need only be represented by a maximal symmetric operator, has obvious implications for the entire matter of quantisation, as exemplified by the radial momentum and time observables. In particular, we could complete Harrison and Wan's model of a current-fed thick superconducting ring by introducing, via the macroscopic wave function hypothesis, maximal symmetric supercurrent operators for the input and output leads. Also, we were able to derive Josephson's equation for a supercurrent that flows through a thin insulating barrier separating two superconductors. Not only was our derivation significantly less ad hoc than the conventional one, but the quantisation method employed may be applied to other systems which possess a circuit configuration.

The self-adjointness requirement for orthodox observables is often relaxed to one of essential self-adjointness [104, p 41]. This is done purely for convenience, as an essentially self-adjoint operator has a unique self-adjoint extension and it is really this extension which is understood to represent the observable. Moreover, an essentially self-adjoint operator possesses a unique orthogonal spectral function and this coincides with the spectral function of its unique self-adjoint extension.

In our theory, a GRI is acceptable as an observable only if it generates a maximal family, or, equivalently, if it is the generalised spectral function of a maximal symmetric operator. Hereafter we refer to such GRIs as *maximal spectral functions.* It turns out that an essentially maximal symmetric operator (a notion we introduced in appendix A) admits a unique maximal spectral function, which generalises the statement that an essentially self-adjoint operator possesses a unique orthogonal spectral function. To see this, suppose $\widehat{A}$ is an essentially maximal symmetric operator, i.e. $\widehat{A}$ is symmetric with a unique maximal symmetric extension that coincides with its closure $\overline{A}$. If $\widehat{A}$ is defined in a Hilbert space $\mathcal{H}$ and $\widehat{F}_\lambda$ is an arbitrary generalised spectral function of $\widehat{A}$ then

$$\langle \psi \mid \widehat{A}\phi \rangle = \int_{-\infty}^{\infty} \lambda d_\lambda \langle \psi \mid \widehat{F}_\lambda \phi \rangle$$

and

$$\left\| \widehat{A}\phi \right\|^2 = \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{F}_\lambda \phi \rangle$$

for all $\psi \in \mathcal{H}$, $\phi \in \mathcal{D}(\widehat{A})$ where $\mathcal{D}(\widehat{A})$ satisfies

$$\mathcal{D}(\widehat{A}) \subseteq \left\{ \phi \in \mathcal{H} : \int_{-\infty}^{\infty} \lambda^2 d_\lambda \langle \phi \mid \widehat{F}_\lambda \phi \rangle < \infty \right\}.$$

If $\widehat{F}_\lambda$ is a maximal spectral function and therefore, by definition, is the generalised spectral function of a maximal symmetric operator $\widehat{B}$ say, then clearly $\widehat{B} \supseteq \widehat{A}$. So, on account of $\widehat{A}$ admitting a unique maximal symmetric extension, we must have $\widehat{B} = \overline{A}$. It follows, by the uniqueness of the generalised spectral function of $\widehat{B}$, that $\widehat{A}$ can have just this one maximal spectral function. Hence an arbitrary essentially maximal symmetric operator possesses a unique maximal spectral function and this is just the generalised spectral function of its unique maximal symmetric extension. In particular, the maximal spectral function of an essentially self-adjoint operator coincides with its orthogonal spectral function.

Wan and Harrison [29] have studied the Josephson effect in a thick superconducting ring (TSCR) containing a single Josephson junction (JJ). In their treatment, the ring, which we shall take as being of unit radius, is identified with the unit circle S^1 where a single point is removed at $\theta = 0$ to signify the presence of the JJ. The ring including the JJ is then identified with the set S^1_o which is isomorphic to the interval $J^o \equiv (0, 2\pi)$. States of the system are taken to be elements of the Hilbert space $L^2(J^o, d\theta)$. The nature of the JJ is built into the Hamiltonian through a momentum dependent cosine term so that Josephson's equation arises from a minimisation of the Hamiltonian eigenvalues. Josephson's equation does not emerge 'naturally' by considering the free-particle Hamiltonian and current operators in $L^2(S^1_o)$ in an analogous fashion to that for the two semi-infinite superconductors separated by a JJ which we considered in section 1.5.2. Indeed, there is no restriction on the current eigenvalues regardless of what the phase across the junction is. Such behaviour is reminiscent of that associated with the 'exceptional Hamiltonians' of section 1.5.2 which we argued were not relevant to the system of two semi-infinite superconductors separated by a JJ. It is puzzling as to why we may derive Josephson's equation for the system of section 1.5.2 in a systematic way but have essentially to put it in by hand for the TSCR system. The situation is even more confusing when one considers a TSCR of large radius, since then the two systems would be indistinguishable in the immediate neighbourhood of the JJ. An obvious difference between the two systems is that the TSCR is a one-component circuit whereas the system of section 1.5.2 is a two-component circuit. Moreover, the phase across the JJ in the TSCR is equally a phase across the bulk of the ring, whereas for the system of section 1.5.2 the phase across the JJ is not equivalent to a phase across the bulk of the superconductor due to the non-finite nature of the components involved. In view of these observations it may be possibe to derive Josephson's equation for the TSCR containing a JJ by a similar method to that in section 1.5.2 if we are able to re-formulate the problem in terms of a multi-component circuit where the phase across the JJ appears in a boundary condition which connects different components of the circuit. As a prospective development, we shall propose an approach which exploits the topology of the ring before the JJ is included.

Consider first a classical particle on S^1. The manifold S^1 is an example of a non-simply connected topological space. This means that not all possible paths which connect two arbitrary points in S^1 are homotopic to one another, i.e. they cannot be continuously deformed into one another [79, pp 242–249]. If, for example, we consider a loop which begins at $\theta = 0$, traverses the circle once and ends at $\theta = 0$, then clearly this is not homotopic to a point at $\theta = 0$. Now to an arbitrary topological space $\mathcal{Q}$ there corresponds a unique universal covering space $\tilde{\mathcal{Q}}$, which is simply connected and has an associated mapping or covering projection, $\pi_{\mathcal{Q}}$, which maps each point in $\tilde{\mathcal{Q}}$ to a unique point in $\mathcal{Q}$. The universal covering space for S^1 is $\mathbb{R}$, and π_{S^1} is given by

$$\mathbb{R} \ni x \longrightarrow \theta = x \; modulo \; 2\pi \in [0, 2\pi).$$

A general universal covering space $\tilde{\mathcal{Q}}$ can be decomposed into a union of 'fundamental domains', each of which is isomorphic to $\mathcal{Q}$. Clearly, we have $\mathbb{R} = \cup_n J_n$ where J_n is the interval $[2n\pi, 2(n+1)\pi)$ which is isomorphic to S^1, and so each J_n is a fundamental domain. A free classical particle moving in S^1 can now be regarded as moving on $\mathbb{R}$ and each time it enters a new fundamental domain this corresponds to it completing another traversal of the circle. If we now remove the point $\theta = 0$ from S^1 to obtain the set S^1_o, then this is equivalent to removing the points $\{2n\pi : n = 0, \pm 1, \pm 2, ...\}$ from $I\!R$ which leaves us with a fragmented covering space $I\!R_o$ given by the union $\cup_n J_n^o$ where $J_n^o = (2n\pi, 2(n+1)\pi)$ and for each n, J_n^o is isomorphic to S_o^1. The particle would then be confined to S_o^1, or, equivalently, to one of the intervals J_n^o. For convenience, we retain the name covering space for $I\!R_o$ and fundamental domain for J_n^o.

In contrast to S_o^1, the covering space $I\!R_o$ forms a multi-component circuit. We would therefore set about quantising on the covering space instead of on S_o^1. For each fundamental domain J_n^o we would introduce a Hilbert space $L^2(J_n^o)$, in which are defined the differential operators $\widehat{P}_n^o \equiv -i\hbar d/dx$ and $\widehat{H}_n^o \equiv -(\hbar^2/2m)d^2/dx^2$ on $C_o^\infty(J_n^o)$. Each of these operators is symmetric with deficiency indices $(1,1)$. Besides the technical difficulties associated with the infinite direct sums which arise in determining momentum ($\Rightarrow$ current) and Hamiltonian operators for the entire system, there is the problem of relating the physics on $I\!R_o$ to the physics on S_o^1. For a related discussion see [105, pp 114–124].

By admitting maximal symmetric operators as observables it becomes possible to rigorise many existing formal quantisation schemes such as those which deal with the quantisation of the momentum in orthogonal curvilinear coordinates. The choice of coordinate system affects the difficulty in quantising the classical momenta on two levels. Firstly, the generally coordinate-dependent volume element which appears in the inner product means that obtaining a momentum operator $\widehat{P}_q$ associated with coordinate q that is even formally symmetric is a non-trivial matter. In particular, we generally do not have $\widehat{P}_q = -i\hbar\partial/\partial q$. This becomes even clearer when one considers the corresponding quantisation of the Hamiltonian (chapter 3). Secondly, the range of the coordinate q is important in determining the uniqueness of the associated maximal symmetric momentum operator $\widehat{P}_q$ and also whether or not $\widehat{P}_q$ is self-adjoint. Generally, if q is of finite range then we obtain uncountably many possible momentum operators and these are all self-adjoint. If q is of semi-infinite range then there corresponds a unique momentum operator and this is maximal symmetric but not self-adjoint. If the range of q is the entire real line then there is a unique momentum operator and it is self-adjoint.

Besides reducing the quantisation problem to essentially one of finding a symmetric operator (all symmetric operators possess maximal symmetric extensions), which can usually be achieved to some extent by purely formal analysis, accepting maximal symmetric operators as observables also extends greatly the applicability of what may be termed adaption schemes, where an already quantised observable is further modified to cater for a specific need. This brings us to chapter 2.

As we remarked in section 2.4.3, allowing maximal symmetric operators to represent observables alleviates some of the difficulties in attributing physical meaning to the local values associated with an unbounded self-adjoint operator $\widehat{A}$. Provided it is densely defined, the operator

$$\widehat{A}_{S_J} \equiv \frac{1}{2}\left\{\widehat{E}(\widehat{X};J)\widehat{A} + \widehat{A}\widehat{E}(\widehat{X};J)\right\}$$

is symmetric and will therefore possess maximal symmetric extensions which may serve as semilocal observables. However, even if $\widehat{A}_{S_J}$ is densely defined, it is generally not possible to express the expectation value of $\widehat{A}$ as a sum over expectation values of semilocal observables for an arbitrary state $\phi \in \mathcal{D}(\widehat{A})$. Since, if $\widetilde{A}_{S_J}$ denotes a maximal symmetric extension of $\widehat{A}_{S_J}$, then there is no guarantee that $\mathcal{D}(\widehat{A})$ will be a subset of $\mathcal{D}(\widetilde{A}_{S_J})$, so the decomposition

$$\langle \phi \mid \widehat{A}\phi \rangle = \sum_i \langle \phi \mid \widetilde{A}_{S_{J_i}}\phi \rangle$$

is generally not valid for all $\phi \in \mathcal{D}(\widehat{A})$. Provided $\cap_i \mathcal{D}(\widetilde{A}_{S_{J_i}})$ is dense then this limitation is not a severe one. Given a $\phi \in \mathcal{D}(\widehat{A})$, it may even be possible to choose a particular set of maximal symmetric extensions of the different $\widetilde{A}_{S_{J_i}}$ so that $\phi \in \cap_i \mathcal{D}(\widetilde{A}_{S_{J_i}})$. We would then have a situation where, for a given partition $\{J_i\}$ of $\boldsymbol{R}$, the state ϕ determines the set $\{\widetilde{A}_{S_{J_i}}\}$ of semilocal observables associated with the observable $\widehat{A}$. We shall now take this idea further and propose a different local values scheme, in which each local value is associated with a weakly local observable that has an explicit state dependence. We shall see that within this new scheme the 'domain problem' does not arise.

Let $\widehat{A}$ be a maximal symmetric operator defined in $L^2(\boldsymbol{R})$ on domain $\mathcal{D}(\widehat{A})$. Given an arbitrary element ϕ of $\mathcal{D}(\widehat{A})$, define the projector $\widehat{P}_\phi$ by $\widehat{P}_\phi \equiv |\phi\rangle\langle\phi|$. We then have the decomposition

$$\langle \phi \mid \widehat{A}\phi \rangle = \sum_i \langle \phi \mid \widehat{A}_\phi^{J_i} \phi \rangle,$$

where

$$\widehat{A}_\phi^{J_i} = \frac{1}{2}\left\{ \widehat{E}(\widehat{X}; J_i)\widehat{P}_\phi \widehat{A} + \widehat{A}\widehat{P}_\phi \widehat{E}(\widehat{X}; J_i) \right\}.$$

Now since $\widehat{P}_\phi \psi \in \mathcal{D}(\widehat{A})$ for all $\psi \in L^2(\mathbb{R})$, then $\widehat{A}\widehat{P}_\phi \widehat{E}(\widehat{X}; J_i)$ is defined on $L^2(\mathbb{R})$. It follows that $\mathcal{D}(\widehat{A}_\phi^{J_i}) = \mathcal{D}(\widehat{A})$ and $(\widehat{A}_\phi^{J_i})^\dagger \supseteq \widehat{A}_\phi^{J_i}$ [61, pp 298–301]. So for each J_i, $\widehat{A}_\phi^{J_i}$ is a symmetric operator and its domain coincides with that of $\widehat{A}$. An appropriate maximal symmetric extension of $\widehat{A}_\phi^{J_i}$ can serve as the relevant observable. Note that $\widehat{A}_\phi^{J_i}$, though weakly local in J_i, is generally not semilocal; this would require $\widehat{P}_\phi \widehat{A} = \widehat{A}\widehat{P}_\phi$. Moreover, the local values $\langle \phi \mid \widehat{A}_\phi^J \phi \rangle$ are different to those of Wan and Sumner. We have

$$\langle \phi \mid \widehat{A}_\phi^J \phi \rangle = \langle \phi \mid \widehat{E}(\widehat{X}; J)\phi \rangle \langle \phi \mid \widehat{A}\phi \rangle,$$

so the local value associated with J is just the product of the 'global value' $\langle \phi \mid \widehat{A}\phi \rangle$ and the probability of finding the system in J, i.e. $\langle \phi \mid \widehat{E}(\widehat{X}; J)\phi \rangle$.

We have seen that the incomplete dynamics associated with non-self-adjoint maximal symmetric Hamiltonians can, by utilising the notion of isometric semigroup, be handled in a mathematically sound way. However, this is not the case in the standard formulation of classical mechanics, where incomplete dynamics corresponds to the equations of motion simply having no solution for $t < 0$ say. So, by allowing maximal symmetric Hamiltonians we are confronted with the question of why we may have a satisfactory quantum description of certain incomplete dynamics but not a satisfactory classical description. In view of Cooper's result that the generalised Schrödinger equation (eqn 3.16) has a solution for all time if and only if the Hamiltonian is self-adjoint, and given the superior description of the evolution in terms of isometric semigroups, it is reasonable to suppose that in a Hilbert space formulation of classical mechanics (see [50, pp 313–318]) incomplete dynamics could also be described in a satisfactory manner by allowing non-self-adjoint maximal symmetric classical Hamiltonians in addition to the self-adjoint ones. Such a generalised formulation of classical mechanics in Hilbert space would provide an extension of the work presented here.

Though our attention was confined to the simplest of functions, we saw, in chapter 3, the necessity of taking maximal symmetric extensions in defining functions of maximal symmetric operators. Take for example the half-line momentum operator $\widehat{P}_{+}$. This is the unique maximal symmetric extension in $L^2(\mathbb{R}^+)$ of the operator $-i\hbar d/dx$ defined on $C_o^\infty(\boldsymbol{R}^+)$. The operator $-(\hbar^2/2m)d^2/dx^2$ defined on $C_o^\infty(\mathbb{R}^+)$ does not, however, possess a unique maximal symmetric extension in $L^2(\boldsymbol{R}^+)$. Instead, we have uncountably many possible energy observables for a free particle on $\boldsymbol{R}^+$, none of which coincides with $(1/2m)\widehat{P}_{+}^2$ since $\widehat{P}_{+}^2$ is not even maximal symmetric. So why is there a unique half-line momentum observable but no unique half-line free-energy observable? In section 3.5.1 we commented on the apparent absorption into the origin of a particle whose evolution was governed by the semigroup $\{T_t^\dagger : t \geq 0\}$ where $\{T_t : t \geq 0\}$ is generated by $-i\widehat{P}_{+}$. We shall now consider the possibility of interpreting this as a real absorption and in so doing "explain" the contrasting uniqueness properties of the half-line momentum and energy observables.

Consider first the various energy observables. These form a one-parameter family $\left\{\widehat{H}_\lambda : \lambda \in \mathbb{R} \cup \{\infty\}\right\}$ of self-adjoint operators in $L^2(\mathbb{R}^+)$ where [50, p 144]:

$$\mathcal{D}(\widehat{H}_\lambda) = \left\{\phi \in L^2(\mathbb{R}^+) : \phi, \phi' \in AC(\mathbb{R}^+), \phi', \phi'' \in L^2(\boldsymbol{R}^+), \phi'(0) + \lambda\phi(0) = 0\right\}$$

$$\mathcal{D}(\widehat{H}_\infty) = \left\{\phi \in L^2(\mathbb{R}^+) : \phi, \phi' \in AC(\boldsymbol{R}^+), \phi', \phi'' \in L^2(\mathbb{R}^+), \phi(0) = 0\right\}$$

and all extensions act on their respective domains as $-(\hbar^2/2m)d^2/dx^2$. A physical interpretation of this non-uniqueness arises if we assume the existence of an infinite potential barrier occupying $x < 0$. The argument runs as follows [50, pp 144–145]. Consider the superposition

$$\phi(x) = e^{-ikx} + \alpha e^{ikx},$$

of an incoming plane wave $exp(-ikx)$ and an outgoing plane wave $exp(ikx)$. Given a $\lambda < \infty$, then ϕ is a generalised eigenfunction of $\widehat{H}_\lambda$ with eigenvalue $\hbar^2k^2/2m$ provided ϕ

is locally in $\mathcal{D}(\widehat{H}_\lambda)$. For this to be the case, we must have $\alpha = (ik - \lambda)/(ik + \lambda)$. The operator $\widehat{H}_\lambda$ is then understood to generate the dynamics in which an incoming plane wave of momentum k is reflected at $x = 0$ by the potential barrier and, since $|\alpha| = 1$, undergoes a phase change of $(ik - \lambda)/(ik + \lambda)$.[6] As the effect of the barrier on the incoming wave depends on λ then the particular choice of self-adjoint extension would be determined by the precise nature of the barrier.

Regarding $\widehat{P}_+$ as a Hamiltonian and thus a generator of dynamics, we may, in view of the above analysis of $\widehat{H}_\lambda$, consider the associated absorption of a wavepacket into the origin as signifying the presence of an infinite thermal reservoir occupying $x < 0$. With this picture, we can perhaps understand why there is only one 'absorption Hamiltonian' but an infinity of 'reflection Hamiltonians'.

Once a particle has been absorbed into an infinite thermal reservoir it can no longer be considered an isolated system. The particle essentially loses its identity and it becomes meaningless to consider its state after absorption. Contrast this with the reflection of a particle by an infinite potential barrier, where it is, of course, meaningful to consider the state of the particle following its encounter with the barrier. The different relative phases between incoming and reflected plane waves of momentum k associated with different barriers are described by different Hamiltonians.

Within this 'literal absorption picture', it may even be possible to reconcile the notions of non-bounded-from-below Hamiltonians and energy observables. Since, by definition, an infinite thermal reservoir is such that the addition or removal of a particle to or from the reservoir does not alter the thermal energy of the reservoir; cf. [2, p 111].

[6] Note that these plane waves are not generalised eigenfunctions of $\widehat{P}_+$. The constraint $\phi(0) = 0$ on states in $\mathcal{D}(\widehat{P}_+)$ is too stringent to allow $\widehat{P}_+$ any generalised eigenfunctions.

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