QUANTUM CHAOS: SPECTRAL ANALYSIS OF FLOQUET OPERATORS

QUANTUM CHAOS: SPECTRAL ANALYSIS OF FLOQUET OPERATORS

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ABSTRACT

The *Floquet operator*, defined as the time-evolution operator over one period, plays a central role in the work presented in this thesis on periodically perturbed quantum systems. Knowledge of the spectral nature of the Floquet operator gives us information on the dynamics of such systems. The work presented here on the spectrum of the Floquet operator gives further insight into the nature of chaos in quantum mechanics. After discussing the links between the spectrum, dynamics and chaos and pointing out an ambiguity in the physics literature, I present a number of new mathematical results on the existence of different types of spectra of the Floquet operator. I characterise the conditions for which the spectrum remains *pure point* and then, on relaxing these conditions, show the emergence of a continuous spectral component. The nature of the continuous spectrum is further analysed, and shown to be *singularly continuous*. Thus, the dynamics of these systems are a candidate for classification as chaotic. A conjecture on the emergence of a continuous spectral component is linked to a long standing number-theoretic conjecture on the estimation of finite exponential sums.

DECLARATION

This is to certify that

(i) the thesis comprises only my original work towards the PhD, except where indicated in the Preface,

(ii) due acknowledgement has been made in the text to all other material used,

(iii) the thesis is less than 100,000 words in length, exclusive of tables, maps, bibliographies and appendices.

James McCaw ________________________________

Date ________________________________

PREFACE

The original work in this thesis has been prepared for publication as follows:

- James McCaw and B. H. J. McKellar. Pure point spectrum for the time evolution of a periodically rank-N kicked Hamiltonian. *J. Math. Phys.*, 46:032108, 2005. Also available at http://arxiv.org/abs/math-ph/0404006. This covers the work presented in Chapter 6.

- James McCaw and B. H. J. McKellar. On the continuous spectral component of the Floquet operator for a periodically kicked quantum system. In preparation. This covers the work presented in Chapter 7.

- J. M. McCaw and B. H. J. McKellar. An analysis of the spectrum for the time evolution of a periodically rank-N kicked Hamiltonian. To appear in the *Proceedings of the AIP National Congress 2005*. This covers the work presented in Chapter 6 and Chapter 7.

Except where explicitly mentioned in the text, this thesis comprises my own work.

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For the uncountably many discussions exploring the concepts, mathematics and peculiarities of chaos in quantum mechanics, thank-you Peter. Your insightful questions helped me clarify ideas and provide improved explanations of much of the work I have done. Without your help, this thesis would not be what it is.

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James McCaw
18th October 2004

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CHAPTER 1

INTRODUCTION

Contents

The main work presented in this thesis is an extension of a number of mathematical results concerning the spectral analysis of time-evolution operators in quantum mechanics for a class of Hamiltonian systems. While the results are of a technical nature and do not lend themselves to a simple "physical" interpretation, they do have potential impacts on the broad field of quantum chaos; specifically the link between the spectrum of an operator[1] and the dynamics of the system.

While this link to quantum chaos turns out to have little impact on the core results presented, it sets the context for the research and drives the course of work

[1]The operator of interest is either the Hamiltonian or the time-evolution operator over one period, depending upon the type of system under consideration.

presented in the two main chapters. I will begin with an investigation of the solutions to the Schrödinger equation when the Hamiltonian is some simple system (e.g., the harmonic oscillator) which is perturbed in a periodic fashion. I will then characterise the spectrum and extend a number of known results in the field of spectral analysis. Along the way, I will build unitary equivalents of a number of well known self-adjoint theorems from functional analysis and discover links between physical conjectures in the physics literature and deep number-theoretic conjectures. The results presented in Chapter 6 and Chapter 7 constitute the main body of research undertaken.

Chapter 2 provides an introduction to both classical and quantum chaos, outlining definitions, techniques and model systems widely used in the literature. Chapter 3 introduces the *Floquet operator*, an essential tool in the investigation of time-periodic quantum mechanical systems.

To discuss the links between dynamics and spectra presented in Chapter 5 properly, an understanding of functional analysis and the mathematics of Hilbert spaces is required. Chapter 4 provides this background, and pointers into the mathematics literature where required. This chapter also develops the background theory and notation used in Chapter 6 and Chapter 7.

As already mentioned, Chapter 5 constitutes a more detailed examination of the literature that motivated my study of the spectrum of operators. I discuss the link between quantum dynamics and spectral analysis of the Hamiltonian operator (time-independent systems) or the time-evolution operator (time-dependent systems). I will also identify a general ambiguity in the literature, pointing out the pitfalls and also a potential resolution to this problem.

1.1 Summary of results

The results of this thesis are presented in detail in Chapter 6 and Chapter 7. I consider systems described by the time-dependent Hamiltonian

$$H(t) = H_0 + \lambda W \sum_{n=0}^{\infty} \delta(t - nT)$$

where H_0 is the time-independent Hamiltonian for some simple system (e.g., the harmonic oscillator), W is an operator describing the perturbation and λ is a strength parameter. The spectral properties of the time-evolution operator over one kick period, T, are investigated.

In Chapter 6 I show that, for arbitrarily strong perturbation strengths λ, the spectrum of the time-evolution operator remains pure point if the perturbation operator W satisfies the condition

$$\sum_n \left| W^{1/2}\phi_n \right| < \infty.$$

The ϕ_n are the basis states of the H_0 system. Essentially, we need $W^{1/2}\phi_n$, when written in terms of the basis states of H_0, to be l_1 convergent.[2] This is a non-perturbative result and indicates that the system described by $H(t)$ is stable—the dynamics does not change in a fundamental way due to the perturbation.

The condition on W is relaxed in Chapter 7 and the possibility for fundamentally different dynamical behaviour is shown to arise in the case where H_0 is the harmonic oscillator, with eigenvalues (ignoring the $1/2\hbar\omega$ term) given by $n\hbar\omega$. When the ratio between the kicking period, T, and the natural frequency, ω, of the unperturbed system is irrational the Floquet operator is shown to obtain a continuous spectral component. This result is proved for rank-N perturbations (i.e., W is

[2] To be a well defined state in the Hilbert space, it must be l_2 convergent. That it is also l_1 convergent is a further restriction which a state in the Hilbert space may or may not satisfy.

a rank-N operator built from N projections), extending the previous rank-1 work of Combescure [28].

The analysis is then extended to the case where H_0 is not the harmonic oscillator, but some general pure point system with eigenvalues described by an arbitrary order polynomial in n (rather than a first order polynomial as is the case for the harmonic oscillator). I show that the question of whether a continuous Floquet spectrum will exist is equivalent to a number-theoretic conjecture presented by Vinogradov [112] over fifty years ago. The conjecture concerns the estimation of Weyl sums—finite sums of the exponential of arbitrary order polynomials. The optimal estimation of such sums for the case where the coefficients of the polynomial are rational is known. For the case where the coefficients are irrational, the current best estimates are not believed to be optimal. Vinogradov's conjecture is that the optimal estimation for such sums is that of the rational coefficient case.

If this conjecture were shown to be true, that is, if such Weyl sums were shown to have a bound given by the rational coefficient case, then the strongest conditions for the existence of a continuous spectrum for the Floquet operator could be established.

The final piece of work presented in Chapter 7 concerns the further classification of the continuous spectrum of the Floquet operator. Extending the results of Milek and Seba [90], I show that the continuous Floquet spectrum is in fact singularly continuous. By the arguments presented in Chapter 5, it is clear that the existence of a singularly continuous component of the Floquet operator is a necessary condition for the time evolution of such systems to show chaotic structure.

CHAPTER 2

CHAOS IN CLASSICAL AND QUANTUM MECHANICS

Contents

The classical study of chaos is now a well established and flourishing field of research in mathematics and mathematical physics. Chaotic behaviour seems to pervade a large number of dynamical systems, and an appreciation of it is essential in many contexts, both applied and theoretical. The classic example of the earth's weather patterns always springs to mind when chaos is mentioned.

The microscopic world, however, is not governed by the laws of classical dynamics. In the realm of small quantum numbers the dynamics of a system is governed by the Schrödinger equation. In such systems, the simple and elegant definitions of chaos such as positive Lyapunov exponent, which hold for classical systems, are not applicable. In fact, there is no universally accepted definition for what constitutes chaos in quantum mechanics. The realisation that the concept of a phase space is not easily translated to quantum mechanics (the uncertainty relation makes it impossible to assign both a position $\vec{x}$ and a momentum $\vec{p}$ simultaneously to a quantum object) immediately precludes a simple link between classical characterisations of chaos and quantum characterisations of chaos. The route past this difficulty is not obvious, and much of the work so far has been centred around finding appropriate tools. As yet, no consensus has been reached on an appropriate definition of *quantum chaos*.

That said, from the early 1980s onwards many papers have been published that adapt classical concepts and bring them into the quantum world. There are also papers that introduce completely new concepts not based on equivalent classical ideas, in an attempt to make sense of quantum dynamics. I will survey some of these ideas in this chapter.

Three broad questions motivate the continued investigation of quantum chaos.

(a) Are there quantum systems that display chaotic behaviour at the quantum level?

(b) What properties of a quantum mechanical system determine whether or not the corresponding classical system will display chaotic behaviour?

(c) Do we come to the same conclusions irrespective of the choice of definitional criteria for quantum chaos?

The first question is very difficult to answer, in part because there is no clear meaning to the expression "chaotic behaviour" when dealing with microscopic phenomena. I will have more to say about this later.

The second question is intimately linked to the *Correspondence Principle* and theories of quantum measurement. It is a generally held belief of physicists (although some do not agree, see [83]) that the classical world is in fact quantum mechanical—how we obtain the classical world from quantum mechanics is a topic of extensive investigation, and needless to say, this area of fundamental physics is infamous for its interpretational difficulties and seemingly inconsistent behaviour. Mixing chaos into the discussion can only make matters more interesting.

The final question is not independent of the previous two, but important to consider when examining the literature. Many attempts to look at particular aspects of the dynamics of quantum systems have been made. They are based around certain toy systems and models. Some papers, as a consequence of their definition of quantum chaos, come to the conclusion that there is no such thing [63]. That is, they conclude that quantum systems do not display chaotic behaviour. Other papers, simply as a result of a different starting point, come to the opposite conclusion. One can certainly say that the pursuits of researchers has uncovered rich variations in the dynamics of simple quantum systems, some of which are now accessible to experiment. New experiments should provide great insight into the numerous models and ideas currently being discussed in the literature. The final word on this exciting field of research is a long way off.

I will now proceed to give an overview of the techniques used in classical and quantum chaos research, and discuss model systems that receive the most attention from the research community. The discussion leads naturally to the new work presented in this thesis on the spectral analysis of unitary operators.

2.1 Chaos in classical systems

The theory of chaos in classical mechanics is well established and understood. The most accessible definition of chaos is obtained from the phase space approach and the growth of the largest Lyapunov exponent for a dynamical system. The path drawn out in phase space $(\vec{x}, \vec{p})$ for a particle is determined by solving the equations of motion. If initially similar phase space points diverge exponentially as time progresses, a Lyapunov exponent for the system is positive, and we say that the system is chaotic. The system displays *sensitivity to initial conditions*. Conversely, systems which only experience power law type separation of trajectories do not have any positive Lyapunov exponents and are deemed non-chaotic.

The Lyapunov exponent definition of chaos is only one of the available characterisations. The famous paper *Period Three Implies Chaos* by Tien-Yien Li and James A. Yorke [87] shows that if a system described by a continuous map[1] has a period of three[2] then it will have periods of all integers and, importantly, also have an uncountable number of initial states which never come even close to being

[1] While Li and Yorke's original paper was concerned with interval maps, it has been extended to the general frame of topological dynamics. See [9].

[2] i.e., After three iterations of the dynamics, we return to the exact initial point

periodic. That is, the evolution of those states never returns to a point arbitrarily close to the initial state.

A third way to characterise chaos in classical systems is to quantify the information required to describe the dynamics of a system. Essentially, if a dynamical system requires an exponentially increasing number of bits to accurately simulate its evolution for a linearly increasing time, then the information content is high, and we say the system is chaotic. If the increase in bits required follows only a power law as the desired time of simulation increases, the system is non-chaotic. Information theory approaches to chaos also include considerations of entropy production in systems. For a beautiful discussion of the links between *unpredictability*, *information* and *chaos*, see [23].

The different characterisations of chaos presented here are believed to be essentially equivalent; attempting to establish this equivalence is an active field of research. As an example, Blanchard *et. al.* [9] have recently shown that the positive entropy characterisation of chaos implies Li–Yorke chaos. For a review of the different approaches to chaos see, for example, the review article by Kolyada and L'. Snoha [81].

In classical mechanics, the simplest model systems in which we observe chaos are iterative, rather than continuous. The logistic map and the Henon-Heiles systems display chaotic behaviour for certain parameter values. Of the continuous systems, the double pendulum is arguably the most elegant example of a chaotic system. The equations of motion are easily solvable, yet the resulting dynamics shows the complexities of chaotic behaviour. Importantly, note that the system is conservative—the total energy is constant over time.

2.2 Kicked systems as a model testing ground for chaos

The field of non-conservative dynamics is a rich one, and chaotic behaviour is a common feature. In particular, it turns out that systems perturbed by an external sharp pulse (a "kick") have interesting dynamical properties. For example, consider a spinning top—a childhood toy. If left to its own devices, it will behave quite predictably, its main axis of rotation precessing slowly, smoothly and *predictably*. There is certainly no chaotic motion. If, however, the spinning top is periodically kicked by a short sharp pulse, the motion turns out to be quite unpredictable; the system is chaotic [57].

This observation has motivated many researchers in the field of quantum chaos to consider quantum systems which are periodically perturbed. They present an attractive combination of physical realisability and mathematical tractability. Featuring strongly in the literature are the kicked rotator (work by Izrailev and Shepelyanskii [71], Grempel and Prange [51], Casati *et. al.* [22], and Dittrich and Graham [37]) and the kicked harmonic oscillator (see Combescure [28], Graham and Hübner [50], and Daly and Hefernan [31]). The quantum kicked top is also examined in great detail by Haake *et. al.* [57,58]. A whole array of other kicked systems have been considered in relation to the study of quantum chaos—see [91,5,4,92] for just some examples. Many of the papers referred to in the next section are also concerned with the analysis of kicked systems.

2.3 Characterisations of quantum chaos

As already mentioned, there is no simple way to take the classical characterisations of chaos and use them in the quantum context. As a consequence, a great deal of research has been done attempting to find appropriate characterisations of quantum systems which provide a clear link to the classical concepts of chaos. In this section, I will review a number of these attempts, highlighting the diversity in the field of quantum chaos. While I separate the discussion into broad sections, this is somewhat artificial. There are significant overlaps between some of the fields. Many of the papers referred to bring together many aspects of quantum chaos.

The paper by Caves and Schack [23], concerning information-theoretic approaches to dynamics, highlights a number of the issues that make the study of chaos so much more difficult in quantum systems, as opposed to the classical systems.

2.3.1 Gutzwiller, periodic orbits and random matrix theory

The field of quantum chaos was arguably born with the work of Gutzwiller [55]. His semi-classical work on calculating the energy eigenvalues for Helium via classical periodic orbits identified the importance of the chaotic nature of the classical dynamics. For more details on his work, see [56, 54]. An excellent review was conducted by Heller and Tomsovic [59]. A few examples of the influence of Gutzwiller's work in the literature is seen in the papers of Eckhardt, Wintgen *et. al.*, Tomsovic and Heller, and Keating [39, 113, 110, 78].

The ideas of Gutzwiller are still of central importance. In an attempt to get to the essence of his work, the study of *quantum billiards* has been developed. Classically, the motion of a particle in a two-dimensional bounded space (such as a billiard table) may be chaotic. The motion is intimately linked to the geometry of the box. By considering a quantum particle constrained to such a geometry, and using Gutzwiller's ideas relating the classical periodic orbits to the quantum energy levels, one can gain great insight into the dynamics of the quantum system.

Importantly, these investigations have also lead to actual experimental investigations in microwave cavities, such as those by Sridhar and Lu, presented in [108] and references therein.

These considerations are intimately related to another technique of great importance in the field of quantum chaos—*random matrix theory*. The eigenvalue statistics of non-chaotic and chaotic systems are, in a sense, *generic*, by which I mean that the energy eigenvalues of chaotic systems typically have the same statistical structure. They are accurately described by random matrix theory—the field of mathematics concerned with the statistics of eigenvalues of classes of random matrices. Billiard systems are an essential tool in work on random matrix theory [13]. See the work of Smilansky [107], Kettemann *et. al.* [79] and the proceedings [26] along with references therein.

2.3.2 de Broglie Bohm theory

Since the initial conception of quantum mechanics, there have been persistent attempts to find a "classical" interpretation of the theory. The dominant *Copenhagen interpretation* of quantum mechanics is most certainly not such an interpretation. The *de Broglie Bohm* interpretation of quantum mechanics [62], largely ignored in the physics community, attempts to provide a strong conceptual link between quantum and classical dynamics; it is based around the Hamilton-Jacobi equations of motion. A quantum particle is just like a classical particle, except that the classical potential it exists in is supplemented by a quantum potential.

The quantum potential is given through the solution of the Schrödinger equation, and thus, results in de Broglie Bohm theory are equivalent to those in standard quantum mechanics.[3] Given that a quantum particle now has a trajectory, a

[3] For over seventy years, this view of the equivalence has prevailed. This is in fact one of the reasons the theory is usually dismissed—it is often seen as nothing more than a rewrite of the

phase space picture of the dynamics is realisable. Thus, both a quantum Lyapunov exponent and hence quantum chaos are definable just as in classical mechanics. The quantum potential blurs the trajectory somewhat, but one can think of a "flux tube" in phase space, describing the evolution of the system.

Papers employing the de Broglie Bohm theory to examine quantum chaos include those by de Alcantara Bonfim *et. al.* [33], de Polavieja [35], Schwengelbeck and Faisal [102, 42], and Wu and Sprung [114]. The de Broglie Bohm theory also plays a central role in a number of the other ideas listed in the following sections.

2.3.3 Open quantum systems

The vast literature on quantum mechanics in open systems also provides a strong link to classical chaos. Tiny environmental interactions which have no effect on the classical systems turn out to be strong enough (easily!) to completely change the quantum dynamics. The coherent interference effects responsible for the "quantum suppression of chaos"[4] are destroyed and the quantum systems show rather classical behaviour, including chaotic behaviour. Fritz Haake's book *Quantum signatures of Chaos* [58] and the many references therein provide an in depth review and excellent discussion of these phenomena. The ideas of Zurek, further discussed by Paz, have also been influential [121, 119, 120, 93]. There has also been experimental work in this area, including the early work of Blümel *et. al.* [11, 10]. On the theoretical side, of interest is much of the work by Cohen, Dittrich *et. al.*, Grobe *et. al.*, and Kohler *et. al.* [25, 37, 38, 52, 80]. The links back

normal quantum theory. However, in recent years there have been some, such as Ghose [47], who claim there are incompatibilities between the theories. Experimentally realisable tests have even been suggested by Golshani and Akhavan [48]. The work is, however, highly controversial and disputed. Struyve and De Baere [109] and other authors referenced therein provide arguments against this suggested incompatibility.

[4] I will detail the meaning of this expression in Section 2.4.

to random matrix theory and level statistics are strong. This work also provides significant insight into Question (b) on page 7.

2.3.4 Other interesting techniques

Here I briefly list a number of other ideas which have been put forward in the literature along with a number of references. Again, many of the ideas draw upon the basic ideas of random matrix theory, de Broglie Bohm theory and open quantum systems.

The Loschmidt echo

A very interesting approach to unifying the concept of chaos in classical and quantum mechanics has been presented by Jalabert and Pastawski [72] and further reviewed by Cucchietti *et. al.* [29]. In classical mechanics, small perturbations in the equations of motion lead to the exponential divergence of trajectories in phase space. It turns out that in quantum mechanics, while small changes to initial conditions do not lead to significantly different dynamical behaviour, small changes in the Hamiltonian can lead to significant variations in the time evolution. The overlap of initially identical wave functions is measured and a Lyapunov exponent is extracted. This recent idea appears promising as it provides an opportunity to directly compare chaotic structure in classical and quantum systems.

The Quantum action

The quantum action was introduced by Jirari *et. al.* [74,75] and utilised by Caron *et. al.* [17,18,19]. The aim is to unify the characterisation of chaos in classical and quantum mechanics by introducing a *quantum action* analogous to the classical action. Jirari *et. al. conjecture* that [75] (quote)

For a given classical action S with a local interaction $V(x)$ there is a renormalized/quantum action

$$\tilde{S} = \int dt \frac{\tilde{m}}{2}\dot{x}^2 - \tilde{V}(x),$$

such that the transition amplitude is given by

$$G(x_{\text{final}}, t_{\text{final}}; x_{\text{init}}, t_{\text{init}}) = \tilde{Z} \exp\left[\frac{i}{\hbar}\tilde{S}\left[\tilde{x}_{\text{class}}\right] \Big|_{x_{\text{init}}, t_{\text{init}}}^{x_{\text{final}}, t_{\text{final}}} \right]$$

where $\tilde{x}_{\text{class}}$ denotes the classical path corresponding to the action $\tilde{S}$.

Note that the mass term, $\tilde{m}$, and the potential, $\tilde{V}$, in the action are quantum parameters. The quantum action takes into account quantum corrections to the classical motion. Once obtained, the tools of classical mechanics may be applied as the mathematical form corresponds exactly with the classical action. The integral is taken only over the classical path.

This direct link allows the definition of chaos in terms of the classical action to be taken over to the quantum dynamics directly.

It must be noted, as acknowledged by Jirari *et. al.* [74], that there is no proof of the conjecture. Numerical evidence is presented by Jirari *et. al.* and Caron *et. al.* that indicates that it seems to be reasonable in a range of cases.

Entropy approaches and information theory

As stated by Słomczyński and Życzkowski in [106], "the approach linking chaos with the unpredictability of the measurement outcomes is the right one in the quantum case". To measure this unpredictability, they introduce a generalised notion of entropy. The inclusion of the measurement process links this approach to some of the open systems work already mentioned. Other papers to recently use an entropy approach include the work by Lahiri [85].

The links between classical chaos and information theory are well known. The ideas can be applied to quantum mechanics too. Some recent work in this field has been done by Inoue *et. al.* [69, 68]. See the references therein for historical details.

Stochastic webs (kicked systems)

The pioneering work of Zaslavskiĭ (see [116, 24] for results and background) investigating the effect of classical phase space structures on quantum dynamics for kicked systems has been fruitful. The ideas of the quantum suppression of chaos are clearly seen in many of these works through an analysis of the diffusive behaviour. See the work by Berman *et. al.*, Borgonovi and Rebuzzini, Chernikov *et. al.*, Daly and Hefernan, Dana, Frasca, Korsch *et. al.*, Sikri and Narchal, Torres-Vega *et. al.*, and Zaslavskiĭ *et. al.* [7,14,24,30,31,32,45,82,103,104,111,118,117] for just a few of the results obtained using these ideas.

2.3.5 Spectral analysis of operators

Finally, as alluded to throughout this review, the analysis of the spectrum of certain operators can be related to the dynamical properties of a quantum mechanical system. I mentioned this when discussing quantum billiards and random matrix theory but it also plays a central role in the examination of kicked systems.

The spectral analysis of operators is a rich mathematical field in its own right and makes numerous claims relevant to the dynamics of quantum systems. The mathematical link between the spectral properties of operators and quantum dynamics is the motivation for the work in this thesis and, accordingly, Chapter 5 is devoted to a fuller exploration of this link.

2.4 Quantum chaos—some established results

Having reviewed some of the broad research areas in quantum chaos, I now briefly present a number of established results from analytic examinations, numerical simulation and experiment that have so far been established. They cut across view points in the field of quantum chaos.

A common property of the time evolution of quantum systems is that for a short time the classical and quantum evolutions correspond. This correspondence is measured by, for example, the energy as a function of time. This is a generic property, and can be attributed to the time it takes for the quantum system to "become aware" of the finite dimensionality of its phase space. After such a time, the correspondence is lost and, while the classical system's energy continues to increase (either in a diffusive way, corresponding to chaotic motion, or in a ballistic fashion, corresponding to resonant energy growth), the quantum system shows recurrences. A great amount of work has been done both analytically and numerically in identifying these timescales. See for example [76, 7, 58, 70].

Related to this is the heuristic link between quantum recurrence and the problem of conduction of electrons in a random lattice—the phenomena of *Anderson localisation*. Again, after a certain time, the classical and quantum evolutions diverge. See [44, 51, 22, 43] for an explanation of the relation between quantum recurrence and Anderson localisation and also the contrast between classical and quantum time evolutions.

The quantum recurrence results are so pervasive that they have lead to a new concept, already mentioned, the *quantum suppression of chaos* [12]. The concept encompasses all these results and reflects the fact that the quantum equivalent of many classically chaotic systems seem to be more well behaved and thus non-chaotic. In a general sense, this behaviour is attributed to the interference effects in the quantum evolution conspiring to suppress dynamical spreading in the wave packets. This take on the results is beautifully explained by Haake [58]. He also shows how the introduction of tiny environmental interactions destroys these interferences effects, leading to rather chaotic-like behaviour for the open quantum systems.

2.5 Summary

I have discussed characterisations of chaos in both classical and quantum theory. While many of the simple ideas from classical mechanics cannot be directly translated into the language of quantum mechanics, there are ways around these problems, e.g., both the de Broglie Bohm theory and the Loschmidt echo approach allow concepts from classical chaos to be brought to the quantum theory.

The "kicked" systems were seen to be of fundamental interest in investigations into quantum chaos, as was the broad field of spectral analysis. Chapter 3 now introduces the basic tools required to consider the quantum evolution of kicked systems.

CHAPTER 3

THE FLOQUET OPERATOR

Contents

The kicked systems are an excellent "testing ground" for chaos in both classical and quantum mechanics. In the quantum case, the time evolution of the system, as governed by the Schrödinger equation, has a particularly elegant form, allowing a stroboscopic analysis of the system to be made. The mathematical tool for this is called the *Floquet operator* and is simply the time-evolution operator over a single kick period. It also goes by the name of *quasi-energy operator* or *monodromy operator* in the literature. The central role that the Floquet operator plays in the work presented in this thesis warrants a detailed introduction, the topic of this chapter. For more information and some simple examples of the Floquet operator, see [58].

3.1 Time evolution in quantum mechanics

The dynamical evolution of a non-relativistic closed quantum system $|\psi(t)\rangle$ is governed by the famous Schrödinger equation,

$$-\frac{i}{\hbar}\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle. \tag{3.1}$$

With this notation, we have a rather simple looking partial differential equation. Of course, this is only an illusion. The vast complexities of quantum mechanics remain hidden.

The formal solution to (3.1) is given by

$$\begin{aligned} |\psi(t)\rangle &= \left[\exp\left(-\frac{i}{\hbar}\int_0^t dt'\, H(t')\right)\right]_+ |\psi(0)\rangle \\ &\equiv U(t,0)|\psi(0)\rangle \end{aligned}$$

where the "+" subscript indicates that we must ensure that the time ordering is done correctly. With correct time ordering, it becomes evident that the relation

$$U(t,0) = U(t,s)U(s,0) \tag{3.2}$$

holds and, due to the unitary nature of the time evolution,

$$U(t,s) = U(t,0)U^\dagger(s,0).$$

Apart from for the simplest of systems such as the harmonic oscillator, square well or the hydrogen atom (and minor variants on them), the Schrödinger equation remains immune to analytic solution. Numerical studies get us some way further, but even then, all but the most simple of experimental situations remain intractable to detailed analysis.

The Hamiltonian $H(t)$ can, in general, be explicitly time dependant, as indicated here. Solutions are just that bit more difficult. In some idealised cases however, there is an effective way to make progress and it turns out to be very useful in the study of potentially chaotic systems. As discussed in Section 2.1, the study of classical systems which experience a periodic (in time) perturbation is of great interest as the motion is often chaotic. If the Hamiltonian is given by some easily solvable system, say a harmonic oscillator or a quantum spinning top or rotor which is then periodically perturbed, the exact solution to the Schrödinger equation can be written down. If

$$H(t) = H_0 + \lambda W \sum_{n=0}^{\infty} \delta(t - nT) \tag{3.3}$$

where H_0 is the time-independent Hamiltonian of the simple system, W is an operator describing the perturbation and λ is a strength parameter, then the solution to the Schrödinger equation at times nT is given by

$$|\psi(nT)\rangle = V^n |\psi(0)\rangle,$$

where I have introduced the so called *Floquet operator* V. V is simply the time-evolution operator for one period T,

$$V \equiv U(T).$$

Using (3.2), the time evolution over one period is

$$V = \exp\left[-\frac{i}{\hbar}\int_{\epsilon}^{T-\epsilon} H(t)\,dt\right] \exp\left[-\frac{i}{\hbar}\int_{T-\epsilon}^{T+\epsilon} H(t)\,dt\right].$$

The first factor, for time $\epsilon \leq t < T - \epsilon$, is trivial. The delta function in (3.3) is not acting, $H(t) = H_0$ is independent of time and the system evolves freely via the time-evolution operator

$$U_0 = e^{-iH_0T/\hbar}.$$

The second factor is over an infinitesimal time period 2ϵ when the delta function kick is acting. Over this infinitesimally short period of time the influence from H_0 is zero. The system instantaneously evolves via the operator

$$e^{-i\lambda W/\hbar}.$$

Recombining these two parts of the evolution, the operator describing the evolution of the system from just before one kick to just before the next is seen to be

$$V = e^{-iH_0T/\hbar}e^{-i\lambda W/\hbar}.$$

At times in this work, I will have need to consider the time-evolution operator taking us from just after one kick to just after the next. By a similar argument, this is given by

$$V' = e^{-i\lambda W/\hbar}e^{-iH_0T/\hbar}.$$

At any rate, they are essentially equivalent—in a given context, one may be more convenient than another. When used, it will always be made clear how the Floquet operator has been defined.

Once the Floquet operator has been obtained, numerical investigations of the system become far more tractable. A stroboscopic picture of the evolution of complex systems can be obtained and investigated. It is also hoped that the idealisation of the delta function pulse is useful when it comes to predicting the behaviour of experimental situations where, for example, a system may be perturbed by a periodic stream of short powerful laser pulses. While each laser pulse clearly interacts with the system over some finite time, the effect on the dynamics should be modelled well by the Floquet operator type "kicks" discussed here.

The Floquet operator also proves useful in analytic work. Specifically, the spectrum of the Floquet operator is of great use in discussing the dynamics of a given quantum mechanical system. Characterisations of the spectrum for particular classes of Hamiltonian systems may be of great value when it comes to predicting how systems behave.

3.2 An example: the kicked top

Here I introduce the simple example of the quantum kicked top to demonstrate the usefulness of the Floquet operator. The analysis is covered in significantly greater detail in the book by Haake [58].

Both the unperturbed Hamiltonian, H_0, and perturbation operator, W, from (3.3) are polynomial functions of the total spin of the top, $\vec{J}$. Conservation of $\vec{J}^2 = j(j+1)$, where I have set $\hbar = 1$ for convenience, implies that the kicked top exists in a finite-dimensional Hilbert space. Choosing, somewhat arbitrarily (but for convenience, see [58]), $H_0 \propto J_x$ and $W \propto J_z^2$ the Floquet operator is simply (c_1 and c_2 are the proportionality constants)

$$V = e^{-ic_1 J_x T} e^{-i\lambda c_2 J_z^2/2j},$$

where the $1/2j$ factor in the instantaneous evolution term is required for the $j \to \infty$ classical limit to make sense. Again, see [58] for a discussion of this.

To proceed, we must specialise to a particular spin system. The spin-$1/2$ system is trivial, so here I briefly describe the spin-1 system. For spin-1 systems, states in the Hilbert space are represented by 3-component spinors (column vectors), and operators by 3×3 matrices which can be decomposed in terms of the Gell–Mann matrices $\lambda_{0,\ldots,8}$. We have $(J_i)_{lm} = -i\hbar\epsilon_{ilm}$ [88], so

$$\begin{aligned} J_z &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= \lambda_2 \end{aligned}$$

and

$$J_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$
$$= \lambda_7.$$

Noting that

$$\lambda_2^2 = 2/3I + \sqrt{3}/3\lambda_8$$

the Floquet operator is

$$V = e^{-ic_1\lambda_7 T} e^{-i\lambda c_2(2/3I+\sqrt{3}/3\lambda_8)/2}$$
$$\equiv e^{-ic_1\lambda_7 T} e^{-ic_3} e^{-ic_4\lambda_8}.$$

where the new constants $c_{3,4}$ have absorbed the various numerical factors and the kicking strength λ. In a numerical study using this operator, the strength is varied by adjusting c_4 appropriately. Note that the term e^{-ic_3} is simply a global phase and hence has no effect on the dynamics.

The final step to be taken is to rewrite the Floquet operator directly as a 3×3 unitary operator. This can be done either analytically or numerically.

Now that we have an appropriate expression for the Floquet operator, the dynamics of a quantum kicked top can now be examined. An initial state, $|\psi_0\rangle$ is chosen

$$|\psi_0\rangle = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$$

and evolved using the matrix representation of the Floquet operator. The resulting states, $|\psi(nT)\rangle$ are given by

$$|\psi(nT)\rangle = V^n|\psi_0\rangle$$

and can be trivially generated numerically for further analysis.

As V is a 3×3 unitary matrix in this case, its spectrum is simply a point spectrum of three eigenvalues.

3.3 Summary

The unitary Floquet operator just introduced provides one with a stroboscopic view of the time evolution of periodically kicked systems. This was demonstrated through the simple example of the spin-1 quantum kicked top. The Floquet operator is the key tool in the work that follows, but in order to understand the work a number of mathematical concepts must first be introduced. These concepts are the topic of Chapter 4.

CHAPTER 4

MATHEMATICAL PRELIMINARIES

Contents

As mentioned in Chapter 3, and to be detailed in Chapter 5, knowledge of the spectrum of the Floquet operator turns out to be important in understanding the dynamics of periodically kicked Hamiltonian systems. To make analytic progress in this field, we will need mathematical tools and concepts that are beyond those usually employed by physicists. In this chapter, I will provide a type of "tutorial" or, if you like, an overview of the fields of measure theory, functional and spectral analysis, picking out those concepts that will be necessary when we come to the work contained in Chapter 6. I begin with a review of integration and measure theory and then proceed to discuss how the concepts of singular, absolute and point measures (to be defined) apply in the context of operators on the physicists' Hilbert space.

4.1 Measure theory

The typical high school introduction to "integration" begins with the idea that the integral of a function gives us the "area under the graph". A suitably well behaved function is split up into smaller and smaller intervals, and each interval approximated by a rectangle, whose height is given by the function evaluated at the mid-point of the interval. The sum of the areas of the rectangles gives an estimation of the area under the function. By taking the limiting case of an infinite number of infinitesimal intervals, the integral of the function is obtained.

This idea of integration is abstracted, formalised and extended to become the Lebesgue integral of modern mathematics [98, 99, 94, 101]. To go beyond this point, the concept of *abstract measure theory* is introduced.

When considering the integral of a function $f(x)$, one usually thinks simply of

$$\int f(x)\, dx$$

where dx is the measure or "size" of an interval. Each interval along the x-axis is given the same weight. An abstraction of this technique is to allow the weight or "size" given to each interval to be determined by a measure function $\alpha(x)$. Any positive, non-decreasing function, $\alpha(x)$ will do. $\alpha(x)$ need not even be continuous. The measure

$$\mu_\alpha([a,b]) = \alpha(b) - \alpha(a)$$

is formed and one obtains the Lebesgue–Steiltjes integral

$$\int_a^b f\, d\mu_\alpha \equiv \int_a^b f\, d\alpha.$$

If $\alpha(x) = x$, we trivially obtain

$$\mu_\alpha([a,b]) = \alpha(b) - \alpha(a) = b - a$$

and recover the usual Lebesgue integral

$$\int_a^b f\, d\alpha = \int_a^b f\, dx.$$

In an intuitive sense, when integrating with respect to a measure function $\alpha(x)$, the contribution to the integral from an interval is proportional to the derivative $d\alpha(x)/dx$. For a given function $\alpha(x)$, if the slope of $\alpha(x)$ is zero for a particular interval, then that interval will contribute nothing, irrespective of the functional value $f(x)$ on that interval.

4.1.1 Point measures

If the measure function is

$$\alpha(x) = \sum_{x'} \theta(x - x')$$

where $\theta(x - x')$ is the usual step-function defined as

$$\theta(x - x') = \begin{cases} 0 \text{ if } x < x', \\ 1 \text{ if } x \geq x' \end{cases}$$

then, in rather loose, but intuitive notation

$$d\alpha(x) = \sum_{x'} \delta(x - x')dx.$$

As we move along the x-axis, we obtain a contribution to the integral $\int f\, d\alpha$ only at the points x'. Each contributing "interval" has a Lebesgue measure of zero—reflected in the fact that in "ordinary integration" the contribution to an integral from a single point is zero, and thus, the occasional infinitely thin but high spike in a function does not matter.

Our integral with the given measure above is now

$$\int f\, d\alpha = \sum_{x'} f(x')$$

and we have converted the integral into a sum.

Measures of this type are called "point measures" for obvious reasons. Compared to integrating a function with respect to the Lebesgue measure, a point measure gives contributions to the integral from single discrete points, exactly where the Lebesgue measure does not contribute. We say that the Lebesgue measure and point measure are *mutually singular*.

4.1.2 Absolutely continuous measures

The absolutely continuous measure is perhaps the simplest of measures apart from the standard Lebesgue measure. If $\alpha(x)$ is a smooth, continuous, everywhere differentiable function of x then we can write

$$\frac{d}{dx}\alpha(x) = g(x)$$

with $g(x)$ continuous and well-behaved. The integral $\int f\, d\alpha$ is then

$$\int f\, d\alpha = \int f(x)g(x)\, dx$$

and we essentially recover the standard Lebesgue integral, but now of the function $f(x)g(x)$ rather than $f(x)$. The absolutely continuous measure satisfies

$$\mu_\alpha([a, b]) = 0 \text{ if and only if } b - a = 0.$$

A simple example is to consider the function $\alpha(x) = (1/2)x^2$. Then $g(x) = x$ and each interval in the integral, instead of having a constant weight, is now weighted by its position on the x-axis.

The absolutely continuous measures are often referred to simply as the continuous measures but I will not do so here, for reasons that will become clear in the following sections.

4.1.3 Singular continuous measures

The point and absolutely continuous measures discussed above are both fairly straight-forward. They quantify concepts that we are already familiar with. However, as is usually the case in mathematics, we can take things further.

It turns out that one can construct measures, μ_α, that contribute to integrals exactly where the Lebesgue measure contributes zero (rather like a point measure), but which are nevertheless continuous measures. This seems contradictory but an example should clarify the idea. We start by defining a particular set, the Cantor set.

Consider the subset S of $[0, 1]$ given by

$$S = \left(\frac{1}{3}, \frac{2}{3}\right) \cup \left(\frac{1}{9}, \frac{2}{9}\right) \cup \left(\frac{7}{9}, \frac{8}{9}\right) \cup \left(\frac{1}{27}, \frac{2}{27}\right) \cup \ldots$$

The Lebesgue measure of S is

$$\frac{1}{3} + 2\left(\frac{1}{9}\right) + 4\left(\frac{1}{27}\right) + \ldots = 1.$$

The complement of this set, $C = [0, 1] \setminus S$, has Lebesgue measure zero and is known as the Cantor set. It contains an infinite number of points but has a size of zero—it is an uncountable set of (Lebesgue) measure 0. See Figure 4.1.

Figure 4.1: The Cantor set

The Cantor function, $\alpha(x)$, is defined by setting

$$\alpha(x) = 1/2 \text{ on } (1/3, 2/3)\,,$$
$$\alpha(x) = 1/4 \text{ on } (1/9, 2/9)\,,$$
$$\alpha(x) = 3/4 \text{ on } (7/9, 8/9)\ldots$$

$\alpha(x)$ becomes a continuous function by continuing this idea all the way to $\alpha(x)$ on $[0, 1]$. The Cantor function $\alpha(x)$ is a non-constant continuous function on $[0, 1]$ whose derivative exists almost everywhere (with respect to the Lebesgue measure) and is zero almost everywhere!

The Cantor function, aptly coined the "Devil's staircase", is shown in Figure 4.2. The function has zero slope almost everywhere, but still manages to rise from 0 to 1 across the finite interval $[0, 1]$ without ever jumping by a finite amount.

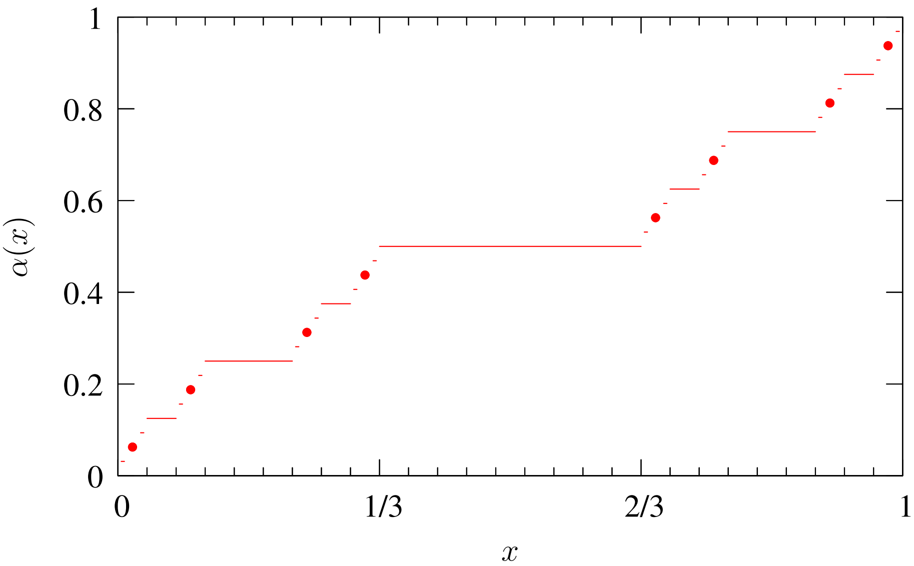

Figure 4.2: The Cantor function

The measure, μ_α, formed using the Cantor function is continuous. That is, $\mu_\alpha(\{p\}) = 0$ for any set $\{p\}$ with only a single point. μ_α contributes to the integral only on the set C, exactly the set on which the normal Lebesgue measure contributes nothing. When integrating with this measure, almost every interval in $[0, 1]$ contributes nothing to the integral as the slope of $\alpha(x)$ is zero almost everywhere.

The Cantor measure is an example of a continuous measure, but one which is mutually singular to the Lebesgue measure. It satisfies

$$\mu_\alpha([a, b]) = 0 \text{ if and only if } b - a \neq 0.$$

Such measures are known as singularly continuous measures.

4.1.4 Summary

I have introduced three types of measure—the point, absolutely continuous and singularly continuous measures. It turns out that an arbitrary measure can always be decomposed into three parts,

$$\mu = \mu_{\text{pp}} + \mu_{\text{ac}} + \mu_{\text{sc}}. \tag{4.1}$$

This decomposition is unique and, importantly, the three pieces are mutually singular. It should be noted that there are other ways to decompose the spectrum into mutually singular parts. While important, in this work I will not have need for such characterisations. The interested reader is referred to [94].

4.2 The tools of functional analysis

Having introduced the notion of a generalised measure of a set on the real line, I now provide an overview of the field of functional analysis, through the introduction of the Hilbert space and operators on the Hilbert space. The abstract measure theory just presented is brought into the picture when discussing the spectral properties of operators on the Hilbert space. It is via this route that the power of functional and spectral analysis enters into mathematical physics. Classifications of the spectrum of operators (the eigenvalues) corresponds to finding the relevant measure to describe the eigenvalues.

Here I only provide a brief overview, defining the pertinent concepts for my work and introducing notation. For a mathematically rigorous, step by step derivation of the concepts discussed, Chapters 1 and 2 in [94] provide an excellent introduction. Much of the chosen notation is inherited from the work of Howland [66]. When, as will sometimes be the case, I need to depart from this notation, I will so indicate.

4.2.1 Hilbert spaces

A vector space which is complete, i.e., one in which all Cauchy sequences converge to an element of the space, is called a *Hilbert space*. The elements of the space are the vectors which physicists use to represent states of a quantum mechanical system. Throughout this work, I will always denote Hilbert spaces by $\mathcal{H}$ or $\mathcal{K}$. Subspaces of a given Hilbert space will often be referred to as $\mathcal{S}$. A Hilbert space is said to be *separable* if and only if it has a countable orthonormal basis. I will only ever consider separable Hilbert spaces in this work. Elements of the space will generally be referenced by either $|\psi\rangle$, $|\phi\rangle$, or in a mathematical, rather than physical context, may often be denoted by x or y.

A subset $\mathcal{S}$ of $\mathcal{H}$ may or may not be complete. The closure of $\mathcal{S}$, $\overline{\mathcal{S}}$ is obtained by adding to $\mathcal{S}$ all the limit points of sequences of elements of $\mathcal{S}$. By closing $\mathcal{S}$, a complete subspace is obtained. A set $\mathcal{S}$ is said to be *dense* in $\mathcal{H}$ if $\overline{\mathcal{S}} = \mathcal{H}$.

The inner product of two vectors $x, y \in \mathcal{H}$ is $\langle x, y\rangle$, and the norm of a vector x is $\|x\| = \langle x, x\rangle^{1/2}$.

4.2.2 Operators

An operator $A : \mathcal{H} \to \mathcal{K}$ acts on elements of the Hilbert space $\mathcal{H}$ and returns elements in the Hilbert space $\mathcal{K}$. It is often the case that $\mathcal{K}$ is either a subspace of, or in fact is, $\mathcal{H}$. Operators on a Hilbert space will always be referenced by uppercase Latin characters.

For an operator $A : \mathcal{H} \to \mathcal{K}$ we define

- the domain $D(A)$; the vectors $x \in \mathcal{H}$ for which Ax is defined,
- the range $R(A) = \{y \in \mathcal{K} : y = Ax \text{ for some } x \in \mathcal{H}\}$,
- the kernel $\ker(A) = \{x \in \mathcal{H} : Ax = 0\}$, and

- the operator norm $\|A\| = \sup_{x \in D(A)\,:\,\|x\|=1} \{\|Ax\|\}$.

An operator is said to be *densely defined* if $R(A)$ is dense in $\mathcal{H}$.

In this work I will have need to consider the family of all operators that can act on a Hilbert space $\mathcal{H}$ and produce an element of $\mathcal{K}$. This space, denoted $\mathcal{L}(\mathcal{H}, \mathcal{K})$ turns out to be a Banach space (a complete normed linear space). The Banach space is a generalisation of a Hilbert space, and thus some of the properties of Hilbert spaces discussed here do not apply to the space of operators. However, many do. Banach spaces will often be denoted by X and Y but context will avoid confusion with operators. See Chapter 3 of [94] for an introduction to Banach spaces.

4.2.3 Invariance and reducing operators

A subspace, $\mathcal{S}$, of $\mathcal{H}$ is called *invariant* for an operator A if, for all $x \in \mathcal{S}$, $Ax \in \mathcal{S}$. That is, action with A on $\mathcal{S}$ does not take us out of $\mathcal{S}$. Further to this definition, a set $\mathcal{S} \in \mathcal{H}$ is said to *reduce* an operator A if both $\mathcal{S}$ and its ortho-complement $\mathcal{H} \ominus \mathcal{S}$ are invariant subspaces for A.

4.2.4 Cyclicity

A vector ϕ is cyclic for an operator A if and only if finite linear combinations of elements of $\{A^n \phi\}_{n=0}^{\infty}$ are dense in $\mathcal{H}$. This motivates the definition that a set $\mathcal{S}$ is cyclic for $\mathcal{H}$ if and only if the smallest closed reducing subspace of $\mathcal{H}$ containing $\mathcal{S}$ is $\mathcal{H}$. This deserves some explanation. The existence of a cyclic vector means that by acting with the operator A and taking linear combinations of the results, the whole Hilbert space $\mathcal{H}$ can be explored. Now consider the reducing subspace $\mathcal{S}$. Action on elements of $\mathcal{S}$ with A always leaves us within $\mathcal{S}$. If repeated operations of this fashion end up reaching all vectors in the full Hilbert space $\mathcal{H}$ (i.e., there are cyclic vectors in $\mathcal{S}$) then the smallest reducing subspace of $\mathcal{H}$ containing $\mathcal{S}$ is $\mathcal{H}$ itself. Hence, the definition above for a set $\mathcal{S}$ to be cyclic corresponds to the existence of at least one cyclic vector in $\mathcal{S}$.

4.2.5 Limits

If A_n is a sequence of operators, s-lim A_n (also $A_n \xrightarrow{s} A$) denotes the strong limit, defined by $\|(A_n - A)g\| \rightarrow 0$ for all $g \in \mathcal{H}$. w-lim A_n (also $A_n \xrightarrow{w} A$) denotes the weak limit, defined by $|\langle A_n g, f\rangle - \langle Ag, f\rangle| \rightarrow 0$ for all $g, f \in \mathcal{H}$. By the Schwartz inequality, the weak limit exists if the condition is satisfied for $f = g$. I will also have need for the norm limit of an operator, $A_n \xrightarrow{n} A$, defined by $\|A_n - A\| \rightarrow 0$.

As the names suggest,

$$A_n \xrightarrow{n} A \Rightarrow A_n \xrightarrow{s} A \Rightarrow A_n \xrightarrow{w} A$$

but the converse need not be true. A trivial application of the Schwartz inequality demonstrates this.

4.3 The spectral theorem

I refer the reader to Chapters 4, 6 and 7 in [94] for a full discussion of the following results. Here I will skip over much of the mathematical detail, only highlighting the pertinent definitions and theorems.

The topic of spectral analysis is essentially an extension of the familiar linear algebra results on matrices of complex numbers to the action of operators on a Hilbert space—the spectrum is constructed in the same way that eigenvalues of a matrix are constructed. Many familiar mathematical expressions and definitions carry over, but great care must be taken to not incorrectly infer results based on those from finite dimensional linear algebra. The change from elements of $\mathbb{C}^n$

to arbitrary vectors in a (possibly infinite dimensional) Banach (or Hilbert) space allows for much more complex behaviour.

I will start by defining the spectrum for an operator $A : X \to X$, mapping elements of the Banach space X into the same space X. The space of such operators $\mathcal{L}(X, X)$ is itself a Banach space. Note that I generalise to consider the operator A acting on a Banach space, rather than a Hilbert space. It is normal practice in the literature to write $\mathcal{L}(X)$ for $\mathcal{L}(X, X)$ when the target space for A is also the initial space. With the spectrum defined, I will then jump ahead to the spectral theorem and the decomposition of the Hilbert space into point, absolutely continuous and singularly continuous reducing subspaces for a particular operator.

4.3.1 The spectrum

Consider $A \in \mathcal{L}(X)$. For $\alpha \in \mathbb{C}$, the operator

$$(\alpha I - A)^{-1}$$

is called the *resolvent* of A at α.

The resolvent set, $\rho(A)$, is defined by

$$\rho(A) = \{\alpha \in \mathbb{C} : (\alpha I - A) \text{ is a bijection with a bounded inverse}\}.$$

If $\alpha \notin \rho(A)$ then α is in the spectrum, $\sigma(A)$, of A. Essentially, the spectrum of A is the set of αs for which the resolvent is not invertible. We now consider an element x of the Banach space X. If there exists an $\alpha \in \mathbb{C}$ such that

$$Ax = \alpha x$$

then x is an *eigenvector* of A and α is the corresponding *eigenvalue*. For now, note that it is possible to have $\alpha \in \sigma(A)$ without α being an eigenvector. See (p. 188, [94]).

4.3.2 Spectral measures

I now specialise to operations on Hilbert spaces. As I will be concerned in this work with unitary operators, I state the following theorems in terms of unitary operators. The literature, however, generally introduces these concepts in terms of self-adjoint operators. As such, the references in this section refer to results on self-adjoint operators, but the results all pass through to unitary operators without much change.

Fix A to be some unitary operator (typically it will be a time-evolution operator) and choose $\psi \in \mathcal{H}$. As discussed in Section VII.2 in [94], one can show that there exists a unique measure, μ_ψ, on the compact set $\sigma(A)$ with

$$\langle \psi, f(A)\psi \rangle = \int_{\sigma(A)} f(\alpha)\, d\mu_\psi. \tag{4.2}$$

The left-hand side of the above equation is a typical inner product that a physicist needs to calculate. On the right-hand side is an integral in the complex plane, which we (hopefully!) have the tools to evaluate. The measure μ_ψ is called the *spectral measure* for the vector ψ. We now begin to see a link between physics and the mathematics presented earlier in Section 4.1. The discussions have lead to a rigorous (although I have not really shown the details) derivation of the common physics practice of evaluating inner products via the insertion of a "complete set of states". The flip-side is that beyond the standard discrete (point) and continuous states found in most physics books, we can now deal with arbitrary measures—point, absolutely continuous and singularly continuous measures.

4.3.3 The spectral theorem

First, I briefly return to the notion of cyclicity introduced earlier. Given an operator A on a separable Hilbert space $\mathcal{H}$, one can always find a decomposition of $\mathcal{H}$

into reducing subspaces

$$\mathcal{H} = \bigoplus_{n=1}^{N} \mathcal{H}_n$$

such that for each subspace $\mathcal{H}_n$ there exists a $\phi_n \in \mathcal{H}_n$ that is cyclic for A restricted to operating on $\mathcal{H}_n$. Note that in the above, N can be finite or countably infinite. See (Lemma 2, p. 226, [94]).

Defining $\mathbb{T}$ to be the unit circle in the complex plane, the spectral theorem states that for a unitary operator, A, on $\mathcal{H}$, there exist measures $\{\mu_n\}_{n=1}^{N}$ ($N = 1, 2, \ldots$ or ∞) on $\sigma(A)$ and a unitary operator

$$U : \mathcal{H} \to \bigoplus_{n=1}^{N} L^2(\mathbb{T}, d\mu_n)$$

such that

$$\left(UAU^{-1}\psi\right)_n(\alpha) = \alpha\psi_n(\alpha)$$

where ψ is a N component vector $(\psi_1(\alpha), \ldots, \psi_N(\alpha)) \in \bigoplus_{n=1}^{N} L^2(\mathbb{T}, d\mu_n)$. Essentially, there exists a unitary operator U that converts operation with A on $\mathcal{H}$ into a linear combination of multiplications by α on elements of the complex unit circle.

After introducing a few more concepts, I will return to another form of the spectral theorem which I will actually use for the rest of this work. It turns out that it is also the most familiar to physicists and provides a strong conceptual link between the mathematics here and the usual treatment of quantum mechanics.

As discussed in Section 4.1, $\mu_{\text{pp,ac,sc}}$ are mutually singular, and thus

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{\text{pp}}) \oplus L^2(\mathbb{R}, d\mu_{\text{ac}}) \oplus L^2(\mathbb{R}, d\mu_{\text{sc}})$$

where I have introduced the space $L^2(\mathbb{R})$, the completion of the space $C(\mathbb{R})$ of real continuous functions.[1] The spectral theorem says that operation with an operator

[1]The completion implies the existence of a metric (or "distance" function). It is simply $\|x - y\|$ for $x, y \in \mathcal{H}$. It is normal practice to drop the measure, $d\mu$, when there can be no confusion, or when it is not necessary for an understanding of the concept being discussed.

A on $\mathcal{H}$ is always equivalent to multiplication operations on the space $L^2(\sigma(A))$ for some appropriate measure μ. Thus, the decomposition of $L^2(\mathbb{R}, d\mu)$ into point, absolutely continuous and singularly continuous parts allows one to conclude that for an operator A acting on $\mathcal{H}$, one can always write

$$\mathcal{H} = \mathcal{H}_{\text{pp}} \oplus \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}}$$

where

$$\begin{aligned}
\mathcal{H}_{\text{pp}} &= \{\psi|\mu_\psi \text{ is pure point}\} = \overline{\{\alpha_n : \alpha_n \text{ is an eigenvalue of } A\}}, \\
\mathcal{H}_{\text{ac}} &= \{\psi|\mu_\psi \text{ is absolutely continuous}\}, \\
\mathcal{H}_{\text{sc}} &= \{\psi|\mu_\psi \text{ is singularly continuous}\}.
\end{aligned}$$

Each subspace reduces the operator A. Introducing the notation $A \restriction \mathcal{H}_{\text{x}}$ for the restriction of A acting only on the subspace $\mathcal{H}_{\text{x}}$, we may conclude that $A \restriction \mathcal{H}_{\text{pp}}$ has a complete set of eigenvectors while $A \restriction \mathcal{H}_{\text{ac}}$ and $A \restriction \mathcal{H}_{\text{sc}}$ have only absolutely continuous and singularly continuous spectral measures respectively.

The pure point, absolutely continuous and singularly continuous spectrum for an operator are now defined by

$$\sigma_{\text{x}}(A) = \sigma(A \restriction \mathcal{H}_{\text{x}}).$$

It is possible to combine the sets in various ways to produce the singular (point plus singular continuous) spectrum and the continuous (absolutely continuous plus singularly continuous) spectrum

$$\begin{aligned}
\sigma_{\text{s}}(A) &= \sigma_{\text{pp}}(A) \cup \sigma_{\text{sc}}(A), \\
\sigma_{\text{cont}}(A) &= \sigma_{\text{ac}}(A) \cup \sigma_{\text{sc}}(A).
\end{aligned}$$

As already alluded to, the form of the spectral theorem above is still not quite what is required in this work. By introducing the concept of *spectral projections* I will now rewrite the spectral theorem in a way that is very familiar to the physicist.

4.3.4 Spectral projections

Section VII.3 in [94] covers the following rigorously as does Chapter VII in [98].

Spectral projections are, intuitively speaking, the building blocks for "operator measures". Just as we considered the integral

$$\int f(x)\, d\alpha(x)$$

and characterised (decomposed) the measure function $\alpha(x)$ in terms of point and continuous measures, here I wish to decompose an operator A on the Hilbert space and write it as

$$A = \int_{\sigma(A)} x\, dE(x)$$

where $E(x)$ is an "operator measure".

The *characteristic function* $\chi_s(x)$ for $S \subset \mathbb{R}$ and $x \in \mathbb{R}$ is defined by

$$\chi_s(x) = \begin{cases} 1 \text{ if } x \in S, \\ 0 \text{ if } x \notin S. \end{cases}$$

The characteristic function provides the foundation for the step-function already introduced in Section 4.1 and is essential in a rigorous development of integration.

The notion of the characteristic function is now extended to operators. To extend the definition, we must first understand how to form functions of operators.

A function of an operator is, in general, defined through a limiting process of polynomials. Just as for functions on the real line, a general function of an operator can be considered as the limit of an appropriate sum of powers of the operator. The characteristic function is just one example. See [98, 94] for the details and the justification for why this formalism is self consistent, i.e., why it makes sense to talk of functions of an operator in this way. Note that this fact is essentially what allowed us to write down (4.2) earlier.

For a unitary operator A and a Borel (think "measurable") set $\Omega \in \mathbb{T}$, the *spectral projection*, $E_\Omega : \mathcal{H} \to \mathcal{H}$ is defined by

$$E_\Omega \equiv \chi_\Omega(A).$$

The spectral projections E_Ω are orthogonal projections as $E_\Omega^2 = E_\Omega$. A family of spectral projections, $\{E_\Omega\}$, has a number of important and rather intuitive properties that mirror the properties of ordinary measures. For a family of sets $\Omega \in \mathbb{T}$, the orthogonal projections have the following properties:

- Each E_Ω is an orthogonal projection,
- $E_\emptyset = 0$; $E_\mathbb{T} = I$,
- If $\Omega = \cup_{n=1}^{\infty} \Omega_n$ with $\Omega_n \cap \Omega_m = \emptyset$ for all $n \neq m$, then
$$E_\Omega = \text{s-}\lim_{N\to\infty} \left(\sum_{n=1}^{\infty} E_{\Omega_n} \right),$$
- $E_{\Omega_n} E_{\Omega_m} = E_{\Omega_n \cap \Omega_m}$.

These properties are exactly those you would expect for a measure—a function that returns the "size" of a set. Any family of projections satisfying the above properties is called a *projection-valued measure* and is, rather confusingly, also denoted by E_Ω, where it is now understood that this is a family of spectral projections, rather than a single spectral projection. As expected, it turns out that for any $\phi \in \mathcal{H}$,

$$\langle \phi, E_\Omega \phi \rangle$$

is just an ordinary measure which one can integrate with respect to. The projections, E_Ω, are self-adjoint[2] and thus $\langle \phi, E_\Omega \phi \rangle$ is real.

[2]Actually, they are *symmetric*. An operator A is symmetric if, for $f, g \in \mathcal{H}$, $(Af, g) = (f, Ag)$. For bounded operators, as considered here, self-adjoint and symmetric are equivalent concepts and hence the use of "self-adjoint" is perfectly acceptable.

Armed with the spectral projections, we can now write an operator (introducing the notation used for the rest of this work), A, simply as[3]

$$A = \int_{\sigma(A)} \alpha \, dE(\alpha) \equiv \int_{\sigma(A)} \alpha E(d\alpha).$$

If A is unitary, then the eigenvalues are on the unit circle in the complex plane, and

$$A = \int e^{-i\theta} E(d\theta).$$

If A is self-adjoint, then

$$A = \int_{-\infty}^{\infty} \alpha E(d\alpha).$$

In the physicist's language, the $E(\alpha)$ are the projections $|\phi_n\rangle\langle\phi_n|$ formed from the eigenvectors $|\phi_n\rangle$ for the operator A. If the eigenvectors are discrete, A is expressed in terms of a sum. If the eigenvectors are continuous[4] then A is written in terms of a standard integral (with measure α the Lebesgue measure).

4.4 Some results and discussion

Having presented most of the concepts and definitions required for the rest of the work, I now summarise a few simple results that will be of use, and discuss some consequences of the theory so far presented.

For any operator, A, the corresponding family $E(\alpha)$ form a general resolution of the identity

$$I = \int E(d\alpha).$$

[3]The subtle change of notation where I have replaced $dE(\alpha)$ with $E(d\alpha)$ is a relic of the development of my work and the conflicting inherited notation from [94] and [66]. In the rest of this work, I generally use the notation $E(d\alpha)$.

[4]We now know that it always eventuated that we had a discrete or absolutely continuous spectrum in the standard physics examples.

Any function of an operator can always be written as

$$f(A) = \int_{\sigma(A)} f(\alpha) E(d\alpha).$$

As the $E(d\alpha)$ are orthogonal projection operators, i.e., $E^2 = E$, we have the very useful result that

$$\int |f(\alpha)|^2 E(d\alpha) = \left| \int f(\alpha) E(d\alpha) \right|^2 .$$

The $E(\alpha)$, being operator measures, can be decomposed into their point, absolutely continuous and singularly continuous components. Thus, we can decompose an operator A into three components: A_{pp}, A_{ac} and A_{sc}. We also form the singular and continuous parts of the operator A,

$$A_{\text{s}} = A_{\text{pp}} + A_{\text{sc}},$$
$$A_{\text{cont}} = A_{\text{ac}} + A_{\text{sc}}.$$

Another minor change in notation due to the way in which this work developed is now introduced. As mentioned earlier in Section 4.2, in a mathematical context I usually use x and y to refer to elements of the Hilbert space $\mathcal{H}$. The ordinary measure formed from a projection-valued measure $E(\alpha)$ for the operator A is now written as m_x, rather than μ_x. I define, for a vector $x \in \mathcal{H}$, the measure

$$m_x(S) = \langle E(S)x, x \rangle$$

where S is a Borel set in $\sigma(A)$. Note that as $E(S)$ is self-adjoint one is free to move it to the other side of the inner product.

Having obtained a full characterisation of operators in terms of their decomposition into point, absolutely continuous and singularly continuous parts, a final definition is now introduced. The operator A is *pure point* if and only if the eigenvectors of A form a basis of $\mathcal{H}$. That is, A is pure point if and only if $\mathcal{H}_{\text{cont}} = \emptyset$ for the operator A.

4.5 Two examples—hydrogen and the harmonic oscillator

To clearly link the preceding discussion back to familiar physics, consider the operator A to be the Hamiltonian, H, for hydrogen and consider the spectrum, σH, of H.

The bound states of hydrogen are a countable number of isolated, discrete energies. Each energy corresponds to an eigenvalue of the system and the set of these points makes up the point energy spectrum. The positive energy scattering states form the continuous energy spectrum. Thus, the energy spectrum for the hydrogen system consists of two disjoint parts: the negative energy discrete (or "point") spectrum, and the positive energy continuous spectrum. For hydrogen, $\sigma_p(H) = \{\alpha_n; \alpha_n \approx -13.6/n^2$ for $n \in \mathbb{N}\}$, and $\sigma_{cont}(H) = (0, \infty)$.

The Hilbert space splits into two subspaces $\mathcal{H}_{\text{pp}}$ and $\mathcal{H}_{\text{cont}} = \mathcal{H}_{\text{ac}}$. There is no singularly continuous component to the Hamiltonian for hydrogen. This is typical of most physics Hamiltonians. The singularly continuous component of an operator is rather abstract and not commonly considered. In certain contexts however, we will see that it becomes an essential tool in obtaining a better understanding of the dynamics of those systems.

As another simple example, the harmonic oscillator quantum system has only discrete energy levels, and thus is said to be "pure point". That is, the eigenvectors of the harmonic oscillator form a basis of the Hilbert Space.

The Hamiltonian of a typical quantum mechanical system does not posses a singularly continuous spectral component and thus, singular continuity is not usually mentioned in texts on quantum mechanics. The physical interpretation of a singularly continuous component to the energy spectrum is murky to say the least.

4.6 Summary

I am now ready to move on and discuss why the spectrum of the Floquet operator is an interesting object to study in the context of quantum chaos. Results on the characterisation of the Floquet operator spectrum in terms of properties of the perturbation to the base Hamiltonian can then be presented.

Chapter 5

Quantum Chaos: The Spectrum of the Floquet Operator

Contents

Having introduced the concept of the Floquet operator in Chapter 3 and the mathematical ideas of measure and spectrum in Chapter 4, I can now bring them together to discuss the dynamics of periodically perturbed quantum systems. One can argue that knowledge of the spectrum of the Floquet operator provides great insight into the dynamics of the system of interest.

The links between spectral decomposition and dynamics is still an active field of research. Model cases provide concrete examples of the links, but the interplay between spectra and dynamics is far from fully understood. Here, I outline the main results and provide references to the current research efforts.

I first consider the case of time-independent systems where the spectrum of the Hamiltonian is important. The RAGE theorem is the starting point for the discussion. Time-dependent systems are then considered—in particular, time-periodic systems whence the Floquet operator's spectrum is of importance when considering the dynamics. The work of Yajima and Kitada [115] on RAGE-like theorems is discussed, as well as the work of Milek and Seba [90]. The important contributions of Antoniou and Suchanecki [2, 3] are also noted. A good overview of the field is provided by Combes [27] and also Last [86]. The introduction in the paper by Enss and Veselić [40] provides the most physically intuitive discussion of the RAGE theorem and is essential reading.

Finally, I also comment on a point of ambiguity seen in a number of papers. I detail the problem in Section 5.3 and suggest a possible reason for why the confusion has survived for nearly twenty years.

5.1 Time-independent systems

For time-independent systems, characterisations of the dynamics is linked to the spectrum of the Hamiltonian through, in part, the RAGE theorem [97]. A large literature considers these systems and the link between dynamics and the spectrum of H. See [86] and the references therein.

A quantum system is characterised by its energy eigenstates, requiring knowledge of the spectrum of H. The time evolution of these states is then examined. Thus, one considers terms like $e^{-iHt}\psi$, where ψ is spectrally decomposed with respect to the operator H.

The RAGE theorem simply states that states in the point subspace, $\mathcal{H}_{\text{pp}}(H)$, survive as time evolves, while states in the continuous subspace, $\mathcal{H}_{\text{cont}}(H)$, decay. Put another way, for systems with a potential, states in the point subspace are *bound states* and essentially remain in a bounded region of space as time evolves. States in the continuous subspace spread in space as time evolves—they are the *scattering states*.

The RAGE theorem is as follows [97]. Let H be a self-adjoint operator and C a compact operator. Then for all $\psi \in \mathcal{H}_{\text{cont}}(H)$,

$$\lim_{T\to\pm\infty} \frac{1}{T} \int_0^T \|C \exp(-itH)\psi\|^2 \; dt = 0.$$

The square on the norm can be dropped by technical considerations [97].

To better understand the RAGE theorem, consider the case where C is a projection, namely [40],

$$C = F(|x| < R).$$

$F(|x| < R)$ is the multiplication operator in x-space with the characteristic function of the ball of radius R. The RAGE theorem then says that for $\psi \in \mathcal{H}_{\text{cont}}(H)$ and a wide class of potentials,

$$\lim_{T\to\pm\infty} \frac{1}{T} \int_0^T \|F(|x| < R) \exp(-itH)\psi\| \; dt = 0$$

for any $R < \infty$. That is, as time evolves, the wave-function ψ has negligible components within an arbitrarily sized ball in space. It spreads to arbitrarily large spatial distances from its initial location.

Conversely, for $\psi \in \mathcal{H}_{\text{p}}(H)$, for all $\epsilon > 0$, there exists an $R(\epsilon)$ such that

$$\sup_{t\in\mathbb{R}} \|F(|x| > R) \exp(-itH)\psi\| < \epsilon.$$

That is, there is some ball of radius R such that the wave-function has negligible components outside that ball for all time. The wave-function remains *localised* in space when $\psi \in \mathcal{H}_{\mathrm{p}}(H)$.

The RAGE theorem provides a course grained overview of the possible dynamics. For $\psi \in \mathcal{H}_{\mathrm{cont}}(H)$ the rate of decay is further dependant upon the characterisation of the continuous spectrum. Singularly continuous states are typically expected to provide the "chaotic" behaviour, sitting somewhere between the ballistic (continuously accelerated) absolutely continuous states and the recurrent point states.

5.2 Time-dependent systems

First and foremost, I refer here to the work by Yajima and Kitada [115]. For systems with a time-periodic Hamiltonian (e.g., kicked systems) a RAGE-like theorem exists, but now the spectrum of interest is that of the Floquet operator, rather than the Hamiltonian.

The numerous discussions on the link between dynamics and the spectrum of H for time-independent systems then apply.

Yajima and Kitada show that for time-periodic systems the Floquet operator spectrum determines the dynamics in the same way that the Hamiltonian spectrum determines the dynamics for time-independent systems.

For time-dependent systems as described in Chapter 3, the following two results [115] apply. The decomposition of the Hilbert space, $\mathcal{H}$, is with respect to the Floquet operator, V. Just as in the work by Enss and Veselić [40], Yajima and Kitada's work [115] is presented in the case where C is the projection operator

$$C = F(|x| < R).$$

For $\psi \in \mathcal{H}_{\text{cont}}(V)$,

$$\lim_{N \to \pm\infty} \frac{1}{N} \sum_{n=0}^{N} \|CV^n \psi\|^2 = 0.$$

For $\psi \in \mathcal{H}_{\text{p}}(V)$, for all $0 < \epsilon < 1$, there exists an $R(\epsilon)$ such that

$$\inf_n \|CV^n \psi\| \geq (1-\epsilon) \|\psi\| .$$

Simply put, for $\psi \in \mathcal{H}_{\text{p}}(V)$, the norm does not decay. After some number of kicks, n, the change in norm is arbitrarily small and the state, initially localised in space, remains localised. The state ψ is a bound state of the system. If $\psi \in \mathcal{H}_{\text{cont}}(V)$ the norm does decay and the state ψ is a scattering state of the system.

The work of Hogg and Huberman [60, 61] takes the point spectrum part of the result one step further. They show that the full wave-function "reassembles" itself infinitely often when the system has a discrete Floquet operator spectrum. The energy also shows recurrent behaviour and the system is seen to be quasi-periodic.

The recurrence of the energy means that for a system to be chaotic, characterised by a diffusive growth in energy, it must have a continuous Floquet spectral component. The exact requirements are a topic of ongoing research. An intuitive discussion is provided by Milek and Seba [90] but it does have its flaws. I discuss this in the next section.

5.2.1 Milek and Seba's work

The singular continuous spectrum of the Floquet operator can, and does, exist in physical systems of interest. With an understanding that Milek and Seba meant to refer to Yajima and Kitada's RAGE-like theorem in [115] rather than the RAGE theorem itself, the argument presented in Section II of their paper [90] shows that if a system possesses a singularly continuous quasi-energy spectrum then its energy growth over time *may* be characteristic of a classically chaotic system. Thus, establishing the existence or otherwise of singular continuous spectra of the Floquet operator is seen to be of central importance to the question of whether or not a quantum mechanical system is chaotic. It must be noted that the arguments presented by Milek and Seba are acknowledged to be anything but rigorous—a point clearly established by Antoniou and Suchanecki [2, 3] who split the singularly continuous spectrum (and of course Hilbert space) into two parts,

$$\mathcal{H}_{\mathrm{sc}} = \mathcal{H}_{\mathrm{sc}}^{\mathrm{Decaying}} \oplus \mathcal{H}_{\mathrm{sc}}^{\mathrm{Non\text{-}decaying}}.$$

The Hilbert space decomposition is reducing. Vectors in the decaying subspace do not survive as $t \to \infty$ while those in the non-decaying subspace do survive. The singular continuous part can act like either a point spectrum or an absolutely continuous spectrum. On reflection, this is to be expected. It is true, as argued by Milek and Seba, that parts of the singularly continuous spectrum will display chaotic behaviour. But there are also parts of the singularly continuous spectrum which do not. The game is wide open in terms of the details and subtleties, but there is no doubt that singularly continuous states can manifest as "chaotic like" behaviour.

With the caveat that the described behaviour is not guaranteed, I now detail the argument of Milek and Seba. It has been inherited from the argument in [22].

Consider the probability $p_{k,l}(n)$ of exciting the k^{th} state of H_0 after n cycles/kicks to the l^{th} state,

$$\begin{aligned} p_{k,l} &= \left|\langle k|V^n|l\rangle\right|^2 \\ &\equiv \left|P_{k,l}(n)\right|^2. \end{aligned}$$

To obtain the probability amplitude $P_{k,l}(n)$ I decompose the Floquet operator V into its point, singularly continuous and absolutely continuous parts. As V is unitary we can write, for ω an eigenvalue,

$$V|\omega\rangle = e^{i\omega}|\omega\rangle.$$

We have

$$p_{k,l} = \left| \int_{\sigma(V)} e^{i\omega n} \langle k | E(d\omega) | l \rangle \right|^2 .$$

Using (4.1) gives three parts,

$$\begin{aligned} P_{k,l} &= \int e^{i\omega n} \, d\mu_{k,l}(\omega) \\ &= \sum_{\sigma_{\text{pp}}(V)} e^{i\omega n} \langle k|\omega\rangle\langle\omega|l\rangle + \int_{\sigma_{\text{ac}}(V)} e^{i\omega n} f_{k,l}(\omega)\, d\omega + \int_{\sigma_{\text{sc}}(V)} e^{i\omega n} \, d\mu_{\text{sc}(k,l)}(\omega). \end{aligned}$$

The transition $k \to l$ will only occur if a state, labelled by ω, links them. That is, for the sum part above, there must be at least one state $|\omega\rangle$ such that $\langle k|\omega\rangle\langle\omega|l\rangle \neq 0$. This demonstrates the importance of the spectral nature of V. If V's spectrum is discrete (only the sum above remains) then the $|\omega\rangle$ states are localised (like δ-function spikes) and hence they can connect only a few states of H_0. In this case one would expect *recurrent behaviour*. As already discussed, this is the essence of Hogg and Huberman's work [60, 61].

If the spectrum is absolutely continuous, the Riemann–Lebesgue lemma (Theorem IX.7, p. 10, [95]) shows that

$$\lim_{n \to \infty} P_{k,l}(n) = 0 \quad \forall k, l.$$

The system is continuously accelerated and we obtain resonant energy growth. This is not chaotic behaviour as the system's future evolution will remain predictable.

If the spectrum of V has a singularly continuous component the possibilities for the dynamics are more varied. The RAGE theorem, as presented in Reed and Simon's book (Theorem XI.115, p. 341, [97]), allows for a very slow diffusive growth in the energy in the presence of a singularly continuous spectral component (p. 343 and Problem 149 on p. 403, [97]).[1] As pointed out by Antoniou

[1]Note that I am referencing the time-independent theory, but as shown by Yajima and Kitada the results flow through to the time-dependent theory which is of interest here.

and Suchanecki [2], this behaviour is not guaranteed—a point which Milek and Seba [90] seem to have missed or at least glossed over. Anyway, it is certainly possible that

$$\lim_{M\to\infty}\sum_{n=0}^{M} p_{k,l}(n) = \infty,$$
$$\lim_{M\to\infty}\frac{1}{M}\sum_{n=0}^{M} p_{k,l}(n) = 0$$

There is a very slow increase in the energy of the occupied state over time. As the first equation diverges we see that the system spends an infinite amount of time in the "lower" states. That is, the system energy does not grow resonantly, but continues to explore the lower energy states as time progresses. The second equation shows, however, that on average the system will eventually escape any fixed chosen state—the system is not bounded in energy.

This slow energy growth (diffusive) behaviour is typical of that seen in classically chaotic systems as mentioned in Chapter 2.

It should be noted that if there is no singularly continuous spectrum, then the diffusive growth described is certainly *not* possible. The existence of a singularly continuous spectrum is a *necessary* condition for chaotic behaviour. It is not a *sufficient* condition.

5.2.2 The quasi-energy self-adjoint operator, K

I have shown in the previous chapters that time-periodic systems are characterised by the Floquet operator—the unitary time-evolution operator over one kick period.

There is an alternative way to access information on the spectral properties and dynamics of such systems. Developed in papers by Howland [64, 65, 67], the self-adjoint quasi-energy operator, or *Floquet Hamiltonian*,

$$K = -id/dt + H(t)$$

turns out to provide a different way to access similar information to what I am seeking from the unitary Floquet operator V. The spectrum of K is directly related to the spectrum of V, as clearly shown in (p. 808, [16]).

K also plays a central role in the work, already discussed, of Yajima and Kitada [115]. To obtain the time-periodic equivalent of the RAGE theorem, Yajima and Kitada first introduce K, apply the original RAGE theorem results, and then convert them into the result on the spectrum of the unitary Floquet operator.

A significant amount of the work on time-dependent systems utilises the Floquet Hamiltonian, K, because, in some sense, working with V proved difficult. The large body of knowledge on self-adjoint operators provides a mature basis for proving theorems about K. As discussed in [16], the spectrum of K is easily related algebraically to that of V, so results on the spectrum for K and V are equivalent.

The trade off is that, especially for a physicist, V is a far more intuitive operator than K. The abstraction involved in working with K must be balanced against the loss of a simple physical picture.

5.3 A point of clarification

It must be noted that the concept of spectrum is associated with a particular operator. Typically, physicists talk of the energy spectrum, associated with the Hamiltonian. However, all operators (e.g., Hamiltonian, Floquet etc.) have a spectrum. A failure to realise, or at the very least to explain, this has lead to a number of potentially misleading papers (see for example [90], but they inherited their argument from [22]) which used results on the spectrum of the Hamiltonian in a discussion of the spectrum of the Floquet operator. While it is probable that the authors are aware of the jump they have made, referring to the work of [115], rather than the original RAGE theorem, would be of significant benefit.

Similarly, papers such as that by Guarneri [53] do not make it clear which operator they are referring to in discussions of the spectrum. The issue is one of language. When physicists refer to "the spectrum" in quantum mechanics, it is generally assumed they mean "the spectrum of the Hamiltonian". That is, the spectrum has come to mean the "energy spectrum" in the language of quantum mechanics. This, however, is not the mathematical definition. The spectrum is associated with a particular operator, as clearly discussed in Chapter 4. This misunderstanding has lead to a number of the more "physical" papers in the literature incorrectly drawing conclusions from the rigorous mathematical literature. It does however turn out that most of the conclusions arrived at are valid. The time-independent system theorems (such as the RAGE theorem) all have equivalent theorems in the time-dependent theory (e.g., the work of Yajima and Kitada, Hogg and Huberman). That no obvious numerical inconsistencies have arisen means that the subtle flaws and potential misunderstandings in the physical literature have gone largely unnoticed for close to twenty years.

I believe that it is of paramount importance that authors exercise great caution when discussing the spectrum of an operator. It should be made clear which operator is being investigated, especially when it is not the Hamiltonian.

The work of Yajima and Kitada [115] is, in this field, the key link due to the fundamental importance of the RAGE theorem for time-independent systems. Unfortunately, it is scantly referenced outside the mathematical literature. Increasing awareness of this important work would be greatly beneficial.

5.4 Summary

It is with the application of the RAGE-like theorem in mind [115], that I undertook the following work on the analysis of the quasi-energy spectrum of the class of Hamiltonians as defined by (3.3). The aforementioned work by Milek and Seba [90], utilising the rank-1 work of Combescure, has shown the manifestation of singularly continuous spectra in numerical simulations of rank-1 kicked rotor quantum systems. The work now presented in Chapter 6 and Chapter 7 extends these results and provides a rigorous mathematical basis to numerical calculations on the time evolution of higher rank kicked quantum systems.

CHAPTER 6

SPECTRAL ANALYSIS OF RANK-N PERTURBED FLOQUET OPERATORS

Contents

This chapter constitutes the first part of the research undertaken in my PhD. The aim is to characterise the spectrum of the Floquet operator for kicked systems as defined by (3.3). The method used parallels the investigation into the spectrum of the Hamiltonian itself undertaken by Howland [66] and relies on the mathematical background presented in Chapter 4. This work is an extension of a result of Combescure [28]. The motivation for investigating the spectrum of the Floquet operator has been discussed in detail in Chapter 5.

6.1 Outline and summary of results

I will derive conditions on the time-periodic perturbations to the base Hamiltonian for the spectrum of the Floquet operator to remain pure point. Equation (3.3) is replaced with a more "technical", but equivalent form,

$$H(t) = H_0 + A^* W A \sum_{n=0}^{\infty} \delta(t - nT), \tag{6.1}$$

where A is bounded, W is self adjoint and H_0 has pure point (discrete) spectrum. In terms of (6.1), the Floquet operator is

$$V = e^{iA^*WA/\hbar} e^{-iH_0 T/\hbar}. \tag{6.2}$$

If A is a rank-1 perturbation,

$$A = |\psi\rangle\langle\psi|$$
$$W = \lambda I$$

then I reproduce the work of Combescure [28]. The vector $|\psi\rangle$ is a linear combination of the orthonormal basis states, $|\phi_n\rangle$, of the unperturbed Hamiltonian H_0

$$|\psi\rangle = \sum_{n=0}^{\infty} a_n |\phi_n\rangle. \tag{6.3}$$

Combescure showed that if $\psi \in l_1(H_0)$, that is if

$$\sum_{n=0}^{\infty} |a_n| < \infty \tag{6.4}$$

then the quasi-energy spectrum remains pure point for almost every perturbation strength λ. I will generalise this result to all finite rank perturbations

$$A = \sum_{k=1}^{N} A_k = \sum_{k=1}^{N} |\psi_k\rangle\langle\psi_k|,$$
$$W = \sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k| \tag{6.5}$$

where $\lambda_k \in \mathbb{R}$ and each vector $|\psi_k\rangle$ is a linear combination of the H_0 basis states, $|\phi_n\rangle$,

$$|\psi_k\rangle = \sum_{n=0}^{\infty} (a_k)_n |\phi_n\rangle. \tag{6.6}$$

The states $|\psi_k\rangle$ are orthogonal,

$$\langle\psi_k|\psi_l\rangle = \delta_{kl}. \tag{6.7}$$

The basic result is that if each $|\psi_k\rangle$ is in $l_1(H_0)$, the spectrum of V will remain pure point for almost every perturbation strength.

The perturbation for which I prove that the quasi-energy spectrum remains pure point is, in fact, more general than the finite rank perturbation presented above. The finite rank result is, however, the motivation for undertaking this work.

Howland [66] showed that the Hamiltonian (6.1) has a pure point spectrum if the ψ_ks are in $l_1(H_0)$. Here I follow a similar argument, showing that the continuous part of the spectrum of V is empty, allowing one to conclude that the spectrum of V must be pure point.

Before proceeding, it should be mentioned that there are alternative routes to results similar to those I present. As mentioned in Section 5.2, associated with the unitary Floquet operator V is the self-adjoint Floquet Hamiltonian K [64]. Utilising K allows the self-adjoint work of Howland [66] to be used directly. This was done by Howland himself [67]. As my work is a unitary equivalent to the work of Howland [66] the results obtained correspond to those determined in [67].

The relationship between my work and Howland's work [66, 67] is similar to the relationship between the self-adjoint rank-1 work of Simon and Wolff [105] and the unitary rank-1 work of Combescure [28].

The techniques developed in this chapter provide new, general theorems applicable to unitary operators and show that it is possible to develop the theory of the spectrum of time-evolution operators directly, without need for the techniques of [64] briefly mentioned earlier in Section 5.2.

In Section 6.2 I will present the main theorems of the chapter, concerned with establishing when systems of the form given by (6.1) maintain a pure point quasi-energy spectrum. Parallelling Howland's paper [66] on self-adjoint perturbations of pure point Hamiltonians, the key ideas are those of U-finiteness and the absolute continuity of the multiplication operator $\mathbb{V}$. To establish the second of these concepts for the unitary case (remember that we are concerned with the spectral properties of the unitary time-evolution operator and not with the spectral properties of the self adjoint Hamiltonian), I will require a modified version of the Putnam–Kato theorem [96]. This, and associated theorems are the topic of Section 6.3. Section 6.4 uses the results of Section 6.2 and Section 6.3 to give the final results, which are then discussed in Section 6.5.

6.2 Spectral properties of the Floquet operator

Let U be a unitary operator on $\mathcal{H}$ and let $\mathcal{K}$ be an auxiliary Hilbert space. Define the closed operator $A : \mathcal{H} \to \mathcal{K}$, with dense domain $D(A)$. For our purposes, A bounded on $\mathcal{H}$ is adequate. I work with a modification (multiplication by $e^{i\theta}$) of the resolvent of U,

$$F(\theta; U) = \left(1 - Ue^{i\theta}\right)^{-1} \tag{6.8}$$

and define for $\theta \in [0, 2\pi)$ and $\epsilon > 0$ the function $G_\epsilon : \mathcal{K} \to \mathcal{K}$,

$$G_\epsilon(\theta; U, A) = AF^*(\theta_+; U)F(\theta_+; U)A^*, \tag{6.9}$$

where $\theta_\pm = \theta \pm i\epsilon$. Let J be a subset of $[0, 2\pi)$.

DEFINITION 6.1 (U-FINITE) *The operator A is U-finite if and only if the operator $G_\epsilon(\theta; U, A)$ has a bounded extension to $\mathcal{K}$, and*

$$G(\theta; U, A) = \operatorname*{s-lim}_{\epsilon \downarrow 0} G_\epsilon(\theta; U, A) \tag{6.10}$$

exists for a.e. $\theta \in J$.

We define the function

$$\begin{aligned} \delta_\epsilon(t) &= \frac{1}{2\pi}\left(\sum_{n=0}^{\infty} e^{in(t+i\epsilon)} + \sum_{n=-\infty}^{0} e^{in(t-i\epsilon)} - 1\right) \\ &= \frac{1}{2\pi}\frac{1 - e^{-2\epsilon}}{1 - 2e^{-\epsilon}\cos(t) + e^{-2\epsilon}}. \end{aligned} \tag{6.11}$$

The limit as $\epsilon \to 0$ of $\delta_\epsilon(t)$ is a series representation of the δ-function. The proof is based on showing that

$$\lim_{\epsilon \downarrow 0} \int_{-\pi}^{\pi} g(t)\delta_\epsilon(t)\, dt = 0$$

where $g(t) = f(t) - f(0)$ and $f(t)$ is bounded in $(-\pi, \pi)$. We split the integral into three parts, $\int_{-\pi}^{-\xi} + \int_{-\xi}^{\xi} + \int_{\xi}^{\pi}$. We must assume that $f(t)$ is continuous at $t = 0$ (otherwise $\int f(t)\delta(t)\, dt$ is not well defined) so that

$$\forall \eta, \exists \xi > 0 \text{ s.t. } \forall t, |t| < \xi \text{ we have } |f(t) - f(0)| < \eta.$$

We have

$$\int_{-\pi}^{\pi} g(t)\delta_\epsilon(t)\, dt = \int_{-\pi}^{-\xi} g(t)\delta_\epsilon(t)\, dt + \int_{-\xi}^{\xi} g(t)\delta_\epsilon(t)\, dt + \int_{\xi}^{\pi} g(t)\delta_\epsilon(t)\, dt. \tag{6.12}$$

Consider the third term in (6.12). For $\xi \leq t \leq \pi$, $\cos t < \cos\xi$, so

$$1 + e^{-2\epsilon} - 2e^{-\epsilon}\cos t \geq 1 + e^{-2\epsilon} - 2e^{-\epsilon}\cos\xi.$$

Therefore

$$\left|\int_{\xi}^{\pi} g(t)\delta_{\epsilon}(t)\,dt\right| \leq \int_{\xi}^{\pi} |g(t)|\,\frac{1}{2\pi}\frac{1-e^{-2\epsilon}}{1-2e^{-\epsilon}\cos\xi + e^{-2\epsilon}}\,dt.$$

Since $g(t)$ is also bounded in $(-\pi,\pi)$, we have

$$|g(t)| \leq K \text{ for } t \in (-\pi,\pi)$$

for some $K \in \mathbb{R}$. Thus,

$$\begin{aligned}\left|\int_{\xi}^{\pi} g(t)\delta_{\epsilon}(t)\,dt\right| &\leq \frac{K}{2\pi}\frac{1-e^{-2\epsilon}}{1-2e^{-\epsilon}\cos\xi + e^{-2\epsilon}}\int_{\xi}^{\pi} dt \\ &\leq \frac{K\pi}{2\pi}\frac{1-e^{-2\epsilon}}{1-2e^{-\epsilon}\cos\xi + e^{-2\epsilon}}.\end{aligned}$$

Taking $\epsilon \to 0$, the denominator

$$1 - 2e^{-\epsilon}\cos\xi + e^{-2\epsilon} \to 2(1-\cos\xi) \neq 0$$

as $\xi > 0$. The numerator $1 - e^{-2\epsilon} \to 0$. Therefore,

$$\left|\int_{\xi}^{\pi} g(t)\delta_{\epsilon}(t)\,dt\right| \to 0 \text{ as } \epsilon \to 0.$$

Similarly, the first term in (6.12),

$$\int_{-\pi}^{-\xi} g(t)\delta_{\epsilon}(t)\,dt \to 0 \text{ as } \epsilon \to 0$$

tends to zero. Now consider the second term in (6.12). We have

$$\left|\int_{-\xi}^{\xi} g(t)\delta_{\epsilon}(t)\,dt\right| \leq \int_{-\xi}^{\xi} |g(t)|\,\delta_{\epsilon}(t)\,dt$$

as $\delta_{\epsilon}(t)$ is a positive function. As $f(t)$ is continuous at $t = 0$, $|g(t)| \leq \eta$ for all $|t| < \xi$, so

$$\begin{aligned}\int_{-\xi}^{\xi} |g(t)|\,\delta_{\epsilon}(t)\,dt &\leq \eta\int_{-\xi}^{\xi} \delta_{\epsilon}(t)\,dt \\ &\leq \eta\int_{\pi}^{\pi} \delta_{\epsilon}(t)\,dt,\end{aligned}$$

where we have again used the positivity of $\delta_\epsilon(t)$ to extend the limits of the integral. This integral is equal to one by ((3.792.1), p. 435, [49]) so we conclude that

$$\left| \int_{-\xi}^{\xi} g(t)\delta_\epsilon(t)\, dt \right| \leq \eta,$$

which can be made as small as desired and thus has the limit zero. We have shown that

$$\lim_{\epsilon\downarrow 0} \int_{-\pi}^{\pi} \left[f(t) - f(0)\right] \delta_\epsilon(t)\, dt = 0.$$

Therefore,

$$\begin{aligned}
\lim_{\epsilon\downarrow 0} \int_{-\pi}^{\pi} f(t)\delta_\epsilon(t)\, dt &= \lim_{\epsilon\downarrow 0} \int_{-\pi}^{\pi} f(0)\delta_\epsilon(t)\, dt + \int_{-\pi}^{\pi} \left[f(t) - f(0)\right] \delta_\epsilon(t)\, dt \\
&= \lim_{\epsilon\downarrow 0} \int_{-\pi}^{\pi} f(0)\delta_\epsilon(t)\, dt \\
&= f(0)
\end{aligned}$$

and we have proved that $\lim_{\epsilon\downarrow 0} \delta_\epsilon(t)$ as defined in (6.11) is an appropriate series representation of the δ-function.

Given (6.11) and the spectral decomposition of U, we may write

$$\begin{aligned}
\delta_\epsilon\left(1 - Ue^{i\theta}\right) &= \int \delta_\epsilon \left(1 - e^{i(\theta-\theta')}\right) E(d\theta') \\
&= \int \delta_\epsilon(\theta - \theta')E(d\theta') \\
&= \frac{1}{2\pi} \int E(d\theta') \left[\sum_{n=0}^{\infty} e^{in(\theta_+ - \theta')} + \sum_{n=0}^{\infty} e^{-in(\theta_- - \theta')} - 1\right] \\
&= \frac{1}{2\pi} \left[\sum_{n=0}^{\infty} e^{in\theta_+} U^n + \sum_{n=0}^{\infty} e^{-in\theta_-} \left(U^*\right)^n - 1\right] \\
&= \frac{1}{2\pi} \left[F(\theta_+; U) + F^*(\theta_+; U) - 1\right] \\
&= \frac{1}{2\pi} \left(1 - e^{-2\epsilon}\right) F^*(\theta_+; U)F(\theta_+; U).
\end{aligned} \tag{6.13}$$

The existence of a non-trivial U-finite operator will have important consequences for the spectrum of the Floquet operator V. We introduce the set

$$N(U, A, J) = \{\theta \in J : \text{s-}\lim_{\epsilon\downarrow 0} G_\epsilon(\theta; U, A) \text{ does not exist}\}$$

of measure zero, which enters the theorem. I will often refer to this set simply as N during proofs.

THEOREM 6.2 *If A is U-finite on J and $R(A^*)$ is cyclic for U, then*

(a) *U has no absolutely continuous spectrum in J, and*

(b) *the singular spectrum of U in J is supported by $N(U, A, J)$.*

Proof. (a) Following Howland, note that the absolutely continuous spectral measure, $m_y^{ac}(J)$, is the $\epsilon \to 0$ limit of $\left\langle \delta_\epsilon \left(1 - Ue^{i\theta}\right) y, y \right\rangle$ for $\theta \in J$. If $y \in \mathcal{H}$ is in $R(A^*)$, allowing one to write $y = A^*x$ for some $x \in \mathcal{K}$, then

$$
\begin{aligned}
&\lim_{\epsilon \downarrow 0} \left\langle \delta_\epsilon \left(1 - Ue^{i\theta}\right) y, y \right\rangle \\
&\quad = \lim_{\epsilon \downarrow 0} \left\langle \delta_\epsilon \left(1 - Ue^{i\theta}\right) A^*x, A^*x \right\rangle \\
&\quad = \lim_{\epsilon \downarrow 0} \frac{\epsilon(1-\epsilon)}{\pi} \left\langle AF^*(\theta_+; U) F(\theta_+; U) A^*x, x \right\rangle \\
&\quad = \lim_{\epsilon \downarrow 0} \frac{\epsilon(1-\epsilon)}{\pi} \left\langle G_\epsilon(\theta; U, A)x, x \right\rangle = 0
\end{aligned}
$$

for a.e. $\theta \in J$. The set $\mathcal{Y}$ of vectors y for which $m_y^{ac}(J) = 0$ is a closed reducing subspace of $\mathcal{H}$, and by construction contains the cyclic set $R(A^*)$ as a subset. Because $\mathcal{Y}$ is invariant, finite linear combinations of action with U^n leaves us in $\mathcal{Y}$. Due to the cyclicity, these same linear combinations allow us to reach any $y \in \mathcal{H}$. Thus, the set $\mathcal{Y}$ of vectors y with $m_y^{ac}(J) = 0$ must be the whole Hilbert space $\mathcal{H}$. So there is no absolutely continuous spectrum of U in J.

(b) A theorem of de la Vallée Pousin ((9.6), p. 127, [101]) states that the singular part of the spectrum of a function is supported on the set where the derivative is infinite. In our case, this corresponds to finding where $m_y(d\theta) \to \infty$. We calculate

$$\lim_{\epsilon\downarrow 0}\langle\delta_\epsilon\left(1-Ue^{i\theta}\right)y,y\rangle = \int\delta(\theta-\theta')\langle E(d\theta')y,y\rangle$$
$$= \int\delta(\theta-\theta')m_y(d\theta')$$
$$= m_y(d\theta).$$

Thus, $m_y^s = m_y^{sc} + m_y^{pp}$ is supported on the set where

$$\lim_{\epsilon\downarrow 0}\left\langle\delta_\epsilon\left(1-Ue^{i\theta}\right)y,y\right\rangle = \infty. \tag{6.14}$$

From the proof to part (a), if $y = A^*x$ then the limit (6.14) is zero for $\theta \in J$, $\theta \notin N$, so m_y^s in J must be supported by N. The set of vectors y with $m_y^s(J\cap N^c) \equiv m_y^s(J\sim N) = 0$ is closed, invariant and contains $R(A^*)$, so must be $\mathcal{H}$ by the argument above. Thus, the singular spectrum of U is supported on the set N. □

Now define a new operator, $Q(z):\mathcal{K}\to\mathcal{K}$,

$$Q(z) = A(1-Uz)^{-1}A^*.$$

Note that

$$Q\left(e^{i\theta_\pm}\right) = AF(\theta_\pm;U)A^*. \tag{6.15}$$

$Q(z)$ is clearly well defined for $|z|\neq 1$. Proposition 6.3 shows that the definition can be extended to $|z|=1$.

PROPOSITION 6.3 *Let A be bounded. If $\theta\in J$, but $\theta\notin N(U,A,J)$, then*

(a) *the operator $Q\left(e^{i\theta}\right) = A\left(1-Ue^{i\theta}\right)^{-1}A^*$ is bounded on $\mathcal{K}$, and*

(b) *one has* $\text{s-}\lim_{\epsilon\downarrow 0} Q\left(e^{\pm i(\theta\pm i\epsilon)}\right) = Q\left(e^{\pm i\theta}\right)$.

Proof. (a) Without loss of generality, take $\theta = 0$ ($z = 1$). By Theorem 6.2, $e^{-i0} \notin \sigma_p(U)$, so $(1 - Ue^{i0})^{-1}$ exists as a densely defined operator. As A is a bounded operator, it suffices to show that $\left(1 - Ue^{i0}\right)^{-1} A^*$ is bounded. We have

$$\begin{aligned} \|\left(1 - Ue^{i0_+}\right)^{-1} A^* x\|^2 &= \langle F(0_+; U)A^*x, F(0_+; U)A^*x\rangle \\ &= \langle AF^*(0_+; U)F(0_+; U)A^*x, x\rangle \\ &= \langle G_\epsilon(0; U, A)x, x\rangle \leq C|x|^2 \text{ (as } \theta \notin N) \end{aligned} \tag{6.16}$$

for some real constant C. If $y = A^*x$, noting $U = \int e^{-i\theta} E(d\theta)$, we also have

$$\|\left(1 - Ue^{i0_+}\right)^{-1} A^* x\|^2 = \int \left(\frac{1}{1 - e^{-i\theta}e^{-\epsilon}}\right)\left(\frac{1}{1 - e^{i\theta}e^{-\epsilon}}\right)\langle E(d\theta)y, y\rangle.$$

In light of (6.16), ϵ may safely be taken to zero to obtain

$$\int \left(\frac{1}{1 - e^{-i\theta}}\right)\left(\frac{1}{1 - e^{i\theta}}\right)\langle E(d\theta)y, y\rangle \leq C\ \|x\|^2 < \infty. \tag{6.17}$$

From (6.17), we have

$$\begin{aligned} &\int \left(\frac{1}{1 - e^{-i\theta}}\right)\left(\frac{1}{1 - e^{i\theta}}\right)\langle E(d\theta)y, y\rangle \\ &\qquad = \left\langle [1 - U]^{-1}y, [1 - U]^{-1}y\right\rangle \leq C\ \|x\|^2 < \infty \end{aligned} \tag{6.18}$$

so $y \in D\left[(1 - U)^{-1}\right]$. Thus, $Q(1) = A(1 - U)^{-1}A^*$ is defined on all $\mathcal{K}$ and bounded.

(b) For $y \in D\left((1 - U)^{-1}\right)$, we show that the difference between $Q\left(e^{\pm i(0 \pm i\epsilon)}\right)$ and $Q\left(e^{\pm i0}\right)$ tends to zero as $\epsilon \to 0$. Again, due to the boundedness of A, we need only show that

$$\|\left(\left(1 - Ue^{i0_+}\right)^{-1} - (1 - U)^{-1}\right) A^* x\|$$

tends to zero. Consider

$$
\begin{aligned}
&\left|\left(1-Ue^{-\epsilon}\right)^{-1}y-(1-U)^{-1}y\right|^2\\
&=\left|\int\left(1-e^{-i\theta}e^{-\epsilon}\right)^{-1}E(d\theta)y-\int\left(1-e^{-i\theta}\right)^{-1}E(d\theta)y\right|^2\\
&=\left|\int\left(\frac{1}{1-e^{-i\theta}e^{-\epsilon}}-\frac{1}{1-e^{-i\theta}}\right)E(d\theta)y\right|^2\\
&=\int\left|\frac{1}{1-e^{-i\theta}e^{-\epsilon}}-\frac{1}{1-e^{-i\theta}}\right|^2\langle E(d\theta)y,y\rangle. \qquad (6.19)
\end{aligned}
$$

To show that this has a limit of zero, write the numerical factor in (6.19) as

$$
\begin{aligned}
\left|\frac{1}{1-e^{-i\theta}e^{-\epsilon}}-\frac{1}{1-e^{-i\theta}}\right|^2&=\left|\frac{e^{-i\theta}\left(1-e^{-\epsilon}\right)}{\left(1-e^{-i\theta}e^{-\epsilon}\right)\left(1-e^{-i\theta}\right)}\right|^2\\
&=\frac{1}{\left(1-e^{i\theta}\right)\left(1-e^{-i\theta}\right)}\left(\frac{\left(1-e^{-\epsilon}\right)^2}{1-2e^{-\epsilon}\cos\theta+e^{-2\epsilon}}\right).
\end{aligned}
$$

Equation (6.19) now equals

$$
\int\left(\frac{\left(1-e^{-\epsilon}\right)^2}{1-2e^{-\epsilon}\cos\theta+e^{-2\epsilon}}\right)\frac{\langle E(d\theta)y,y\rangle}{\left(1-e^{-i\theta}\right)\left(1-e^{i\theta}\right)}. \qquad (6.20)
$$

The first factor is bounded and tends to zero for $\theta\neq 0$. The second factor is the measure from (6.17). Clearly, away from the origin, the integral tends to zero. About the origin, some care must be taken to show that there is no contribution to the integral.

Using (6.11), we have

$$
\frac{\left(1-e^{-\epsilon}\right)^2}{1-2e^{-\epsilon}\cos\theta+e^{-2\epsilon}}=\frac{\left(1-e^{-\epsilon}\right)^2}{1-e^{-2\epsilon}}2\pi\delta_\epsilon(\theta).
$$

On substitution into (6.20), we obtain

$$
\frac{\left(1-e^{-\epsilon}\right)^2}{1-e^{-2\epsilon}}2\pi\int_{-\alpha}^{\alpha}\delta_\epsilon(\theta)\frac{m_y(d\theta)}{2(1-\cos\theta)}=\frac{\left(1-e^{-\epsilon}\right)^2}{1-e^{-2\epsilon}}2\pi\int_{-\alpha}^{\alpha}\frac{d\Theta_\epsilon}{d\theta}\frac{g_y(\theta)}{2(1-\cos\theta)}\,d\theta.
$$

The function $\Theta_\epsilon(\theta)=\int\delta_\epsilon(\theta')\,d\theta'$ is the step function in the $\epsilon\to 0$ limit. For non–zero ϵ it is positive, monotonic, increasing and bounded by unity. As $\theta\notin N$

I have also written $m_y(d\theta) = g_y(\theta)d\theta$ for some well behaved positive function $g_y(\theta)$. By integration by parts (see p. 32, [73] for existence conditions, which are satisfied) we obtain

$$\frac{(1-e^{-\epsilon})^2}{1-e^{-2\epsilon}}2\pi\left\{\left[\Theta_\epsilon(\theta)\frac{g_y(\theta)}{2(1-\cos\theta)}\right]_{-\alpha}^{\alpha} - \int_{-\alpha}^{\alpha}\Theta_\epsilon(\theta)\frac{d}{d\theta}\frac{g_y(\theta)}{2(1-\cos\theta)}\,d\theta\right\}.$$

The first term within the curly braces is clearly some finite value. The second term is less than

$$\int_{-\alpha}^{\alpha}\frac{d}{d\theta}\frac{g_y(\theta)}{2(1-\cos\theta)}\,d\theta = \left[\frac{g_y(\theta)}{2(1-\cos\theta)}\right]_{-\alpha}^{\alpha}$$

from the properties of the Θ_ϵ function mentioned above. As with the first term, it is clearly some finite value. Noting that

$$\lim_{\epsilon\downarrow 0}\frac{(1-e^{-\epsilon})^2}{1-e^{-2\epsilon}} = 0,$$

part (b) follows. □

THEOREM 6.4 *Let A be bounded and U-finite on J, with $R(A^*)$ cyclic for U. Let W be bounded and self-adjoint on $\mathcal{K}$, and define the Floquet operator,*

$$V = e^{iA^*WA/\hbar}U.$$

Assume that for $|z| \neq 1$, $Q(z)$ is compact, and that $Q\left(e^{\pm i(\theta \pm i\epsilon)}\right)$ converges to $Q\left(e^{\pm i\theta}\right)$ in operator norm as $\epsilon \to 0$ for a.e. θ in J. Define the set

$$M(U,A,J) = \{\theta \in J : Q\left(e^{\pm i(\theta \pm i0)}\right) \text{ does not exist in norm}\}.$$

Then

(a) *V has no absolutely continuous spectrum in J, and*

(b) *the singular continuous part of the spectrum of V in J is supported by the set $N(U,A,J) \cup M(U,A,J)$.*

Proof. (a) For convenience, write the Floquet operator as

$$V = (1 + A^*ZA)U,$$

where Z is defined appropriately by requiring[1] $\exp(iA^*WA/\hbar) = 1 + A^*ZA$. Noting (6.8) and (6.15) allows one to define

$$\begin{aligned} Q_1\left(e^{i\theta}\right) &= AF(\theta; V)A^* \\ &= A\left(1 - Ve^{i\theta}\right)^{-1} A^*. \end{aligned}$$

Consider some vector $y' \in \mathcal{H}$. $Ay' = x \in \mathcal{K}$ is defined for such y'. $A^*x = y''$ is some vector in $\mathcal{H}$. The cyclicity of $R(A^*)$ means that action with linear combinations of powers of U on y'' allows one to obtain any $y \in \mathcal{H}$, the original y' being one of them. Thus, we have a construction of A^{-1}, namely, operation with A^* followed by the linear combination of powers of U. As y' was arbitrary, A^{-1} exists for all $y \in \mathcal{H}$. This allows one to introduce $I = A^{-1}A$ in what follows.[2]

We now proceed by use of the resolvent equation,

$$\begin{aligned} &Q_1 - Q \\ &\quad = A\left\{\frac{1}{1 - Ve^{i\theta}} - \frac{1}{1 - Ue^{i\theta}}\right\} A^* \\ &\quad = A\left\{\frac{1}{1 - Ve^{i\theta}}(V - U)e^{i\theta}\frac{1}{1 - Ue^{i\theta}}\right\} A^* \\ &\quad = A\left\{\frac{1}{1 - Ve^{i\theta}}\left([1 + A^*ZA - 1]Ue^{i\theta}\right)\frac{1}{1 - Ue^{i\theta}}\right\} A^* \\ &\quad = A\left\{\frac{1}{1 - Ve^{i\theta}}\left(A^*ZAUe^{i\theta}\right)\frac{1}{1 - Ue^{i\theta}}\right\} A^* \\ &\quad = Q_1\left(e^{i\theta}\right) ZAUA^{-1}e^{i\theta}Q\left(e^{i\theta}\right). \end{aligned} \tag{6.21}$$

[1] For the rank-N perturbation case where $W = \sum_{k=1}^{N} \lambda_k|\psi_k\rangle\langle\psi_k|$ and $A = \sum_{k=1}^{N} |\psi_k\rangle\langle\psi_k|$, we have $Z = \sum_{k=1}^{N}(\exp(i\lambda_k/\hbar) - 1)|\psi_k\rangle\langle\psi_k|$.

[2] The particular choice of A as a projection in (6.5) does not have an inverse, but I will show in Section 6.4 that one can define a subspace of $\mathcal{H}$ on which $R(A^*)$ is cyclic, and apply this theorem.

Thus, briefly using $L = ZAUA^{-1}e^{i\theta}$ for clarity, we have

$$\begin{aligned} LQ_1 - LQ &= LQ_1 LQ \\ \Rightarrow \qquad 1 - LQ + LQ_1 - LQ_1 LQ &= 1 \\ \Rightarrow \qquad (1 + LQ_1)(1 - LQ) &= 1 \\ \Rightarrow \qquad 1 + e^{i\theta} ZAUA^{-1} Q_1 \left(e^{i\theta}\right) &= \\ \left[1 - e^{i\theta} ZAUA^{-1} Q\left(e^{i\theta}\right)\right]^{-1}. \end{aligned} \tag{6.22}$$

Denote by N and M the sets $N(U, A, J)$ and $M(U, A, J)$. If $\theta \in (J \sim N) \sim M$, i.e., $\theta \in J \cap N^c \cap M^c$, and $1 - e^{i\theta} ZAUA^{-1} Q\left(e^{i\theta}\right)$ is not invertible, then the compactness of $-LQ\left(e^{i\theta}\right)$ (which follows from the compactness of $Q\left(e^{i(\theta+i\epsilon)}\right)$, the norm convergence of $Q\left(e^{i(\theta+i\epsilon)}\right)$ and (Theorem VI.12, [94])) allows one to use the Fredholm Alternative (Theorem VI.14, p. 201, [94]) to assert that

$$\exists x \in \mathcal{K}, \text{ s.t. } \left[1 - e^{i\theta} ZAUA^{-1} Q\left(e^{i\theta}\right)\right] x = 0.$$

That is, there is some vector $x \in \mathcal{K}$ which satisfies the equation

$$x - e^{i\theta} ZAUA^{-1} A \left(1 - Ue^{i\theta}\right)^{-1} A^* x = 0. \tag{6.23}$$

As $\theta \in J \sim N$, by Proposition 6.3 $y = A^* x \in D\left[\left(1 - Ue^{i\theta}\right)^{-1}\right]$ so define ϕ as

$$\phi = \left(1 - Ue^{i\theta}\right)^{-1} A^* x. \tag{6.24}$$

ϕ is a well defined vector on $\mathcal{H}$ and we have

$$x - e^{i\theta} ZAU\phi = 0,$$

which implies that

$$x = e^{i\theta} ZAU\phi.$$

By (6.24), $x \neq 0$ implies $\phi \neq 0$, so we have

$$\left(1 - Ue^{i\theta}\right)\phi = A^*x = e^{i\theta}A^*ZAU\phi,$$

whence

$$(1 + A^*ZA)\,U\phi = e^{-i\theta}\phi,$$

or

$$V\phi = e^{-i\theta}\phi. \tag{6.25}$$

We conclude that $e^{-i\theta} \in \sigma_p(V)$.

The multiplicity of the eigenvalue is given by the dimension of the kernel of $1 - e^{i\theta}ZAUA^{-1}Q$, which is finite by the compactness of Q and (Theorem 4.25, [99]).

Therefore, if $\theta \in J \sim (N \cup M \cup \sigma_p(V))$, which is a set of full Lebesgue measure,[3] then the vector

$$\begin{aligned} x(\epsilon) &= \left[1 + e^{i(\theta+i\epsilon)}ZAUA^{-1}Q_1\left(e^{i(\theta+i\epsilon)}\right)\right]x \\ &\equiv \left[1 + L_+Q_1\left(e^{i\theta_+}\right)\right]x \end{aligned} \tag{6.26}$$

must be bounded in norm as $\epsilon \to 0$ because we have just seen that if it is unbounded we have an eigenvalue of the operator V. For $y = A^*x \in R(A^*)$, the absolutely continuous spectrum, m_y^{ac}, of V is the limit of

$$\left\langle \delta_\epsilon\left(1 - Ve^{i\theta}\right)y, y\right\rangle = \left\langle A\delta_\epsilon\left(1 - Ve^{i\theta}\right)A^*x, x\right\rangle.$$

The aim is to show that this is zero for all $y \in \mathcal{H}$. Define

$$F_1(\theta) = \left(1 - Ve^{i\theta}\right)^{-1}, \tag{6.27}$$

$$F(\theta) = \left(1 - Ue^{i\theta}\right)^{-1} \tag{6.28}$$

and in a similar fashion to (6.21) and (6.22), we obtain

$$F_1(\theta) = F(\theta)\left[1 + (V - U)e^{i\theta}F_1(\theta)\right] \tag{6.29}$$

[3] That the set M has measure zero is a consequence of Lemma 6.5 on page 79.

and

$$\left(1+(V-U)e^{i\theta}F_1(\theta)\right)=\left(1-(V-U)e^{i\theta}F(\theta)\right)^{-1}.$$

Writing $X=V-U$, on substituting (6.29) into the expression for the δ-function (6.13) we obtain

$$\begin{aligned}2\pi\delta_\epsilon\left(1-Ve^{i\theta}\right)&=\left(1-e^{-2\epsilon}\right)F_1^*(\theta_+)F_1(\theta_+)\\&=\left[1+e^{i\theta_+}XF_1(\theta_+)\right]^*2\pi\delta_\epsilon\left(1-Ue^{i\theta}\right)\left[1+e^{i\theta_+}XF_1(\theta_+)\right].\end{aligned}$$

Substitution of (6.15) and noting that

$$X=V-U=(1+A^*ZA)U-U=A^*ZAU$$

gives

$$\begin{aligned}&A\delta_\epsilon\left(1-Ve^{i\theta}\right)A^*\\&\quad=A\left[1+Xe^{i\theta_+}F_1(\theta_+)\right]^*\delta_\epsilon\left(1-Ue^{i\theta}\right)\left[1+Xe^{i\theta_+}F_1(\theta_+)\right]A^*\\&\quad=A\left[1+e^{-i\theta_-}F_1^*(\theta_+)U^*A^*Z^*A\right]\delta_\epsilon\left(1-Ue^{i\theta}\right)\left[1+e^{i\theta_+}A^*ZAUF_1(\theta_+)\right]A^*\\&\quad=\left[A+e^{-i\theta_-}AF_1^*(\theta_+)A^*\left(A^*\right)^{-1}U^*A^*Z^*A\right]\delta_\epsilon\left(1-Ue^{i\theta}\right)\\&\qquad\qquad\times\left[A^*+e^{i\theta_+}A^*ZAUA^{-1}AF_1(\theta_+)A^*\right]\\&\quad=\left[1+e^{-i\theta_-}Q_1^*(\theta_+)\left(A^*\right)^{-1}U^*A^*Z^*\right]A\delta_\epsilon\left(1-Ue^{i\theta}\right)A^*\\&\qquad\qquad\times\left[1+e^{i\theta_+}ZAUA^{-1}Q_1(\theta_+)\right]\\&\quad=\left[1+L_+Q_1(\theta_+)\right]^*A\delta_\epsilon\left(1-Ue^{i\theta}\right)A^*\left[1+L_+Q_1(\theta_+)\right].\end{aligned}$$

The absolutely continuous spectrum, m_y^{ac} of V is the $\epsilon\to 0$ limit of

$$\begin{aligned}&\left\langle A\delta_\epsilon\left(1-Ve^{i\theta}\right)A^*x,x\right\rangle\\&\quad=\left\langle\left[1+L_+Q_1(\theta_+)\right]^*A\delta_\epsilon\left(1-Ue^{i\theta}\right)A^*\left[1+L_+Q_1(\theta_+)\right]x,x\right\rangle\\&\quad=\left\langle A\delta_\epsilon\left(1-Ue^{i\theta}\right)A^*x(\epsilon),x(\epsilon)\right\rangle\\&\quad=\frac{\epsilon(1-\epsilon)}{\pi}\left\langle G_\epsilon(\theta;U,A)x(\epsilon),x(\epsilon)\right\rangle\end{aligned}\tag{6.30}$$

which tends to zero as $\epsilon \to 0$ if both $G_\epsilon(\theta; U, A)$ and $x(\epsilon)$ are bounded. $G_\epsilon(\theta; U, A)$ is bounded as $\theta \in J \sim N$ and $x(\epsilon)$ is bounded by (6.26).

Part (a) follows since $R(A^*)$ cyclic for U implies that $R(A^*)$ is cyclic for V.

(b) Let $N_1 = N(V, A, J)$. We have just shown that $\theta \in J \sim (N \cup M \cup \sigma_p(V))$ implies that

$$\frac{\epsilon}{\pi} \langle G_\epsilon(\theta; V, A) x(\epsilon), x(\epsilon) \rangle \to 0 \tag{6.31}$$

and therefore

$$\langle \delta_\epsilon \left(1 - V e^{i\theta}\right) y, y \rangle \to 0. \tag{6.32}$$

If we can infer the strong limit from this weak limit then we have established that $\theta \notin N_1$. We use the result that if $x_n \overset{w}{\to} x$ and $\|x_n\| \to \|x\|$, then $x_n \overset{s}{\to} x$ ([6], p 244). Writing G_ϵ and G for $G_\epsilon(\theta; V, A)$ and $G(\theta; V, A)$, and F_ϵ and F for $F(\theta_+; V)$ and $F(\theta; V)$, consider

$$\begin{aligned}
&\left| \|G_\epsilon x\|^2 - \|Gx\|^2 \right| \\
&\qquad = \left| \langle (G_\epsilon^2 - G^2) x, x \rangle \right| \\
&\qquad = \left| \langle A \left\{ \left(F_\epsilon^* F_\epsilon - F^* F\right) A^* A F_\epsilon^* F_\epsilon + F^* F A^* A \left(F_\epsilon^* F_\epsilon - F^* F\right) \right\} A^* x, x \rangle \right| .
\end{aligned}$$

If A, F_ϵ and F are bounded operators, then if $F_\epsilon^* F_\epsilon - F^* F$ tends to zero as $\epsilon \to 0$ we can conclude that the strong limit exists. A short calculation shows that

$$F_\epsilon^* F_\epsilon - F^* F = \left[\left(1 - e^{-2\epsilon}\right) - \left(1 - e^{-\epsilon}\right) \left(U e^{i\theta} + U^* e^{-i\theta}\right) \right] F_\epsilon^* F_\epsilon F^* F$$

which trivially tends to zero as $\epsilon \to 0$ given the boundedness of F_ϵ and F. Finally, A is bounded by assumption and (6.26) shows that $Q_1(\theta_+)$ is a bounded operator as $\epsilon \to 0$ and thus both F_ϵ and F are bounded.

Moving on from (6.32), we have now established that $N_1 \subset N \cup M \cup \sigma_p(V)$ so N_1 must have measure zero, again remembering that we need Lemma 6.5 below to prove that M has measure zero. By Theorem 6.2, N_1 supports the singular spectrum of V. That is,

$$m^s\left(N_1^{\mathrm{c}}\right) = 0$$

where the set N_1^{c} is the complement of N_1. As the measure is positive and $m^s = m^{sc} + m^p$, we know that

$$m^{sc}\left(N_1^{\mathrm{c}}\right) = 0.$$

Trivially, $(N \cup M) \sim \sigma_p(V)$ contains $N_1 \sim \sigma_p(V)$. Thus

$$\begin{aligned} m^{sc}\left([N_1 \cap \sigma_p(V)^{\mathrm{c}}]^{\mathrm{c}}\right) &= m^{sc}\left(N_1^{\mathrm{c}} \cup \sigma_p(V)\right) \\ &= m^{sc}\left(N_1^{\mathrm{c}}\right) + m^{sc}\left(\sigma_p(V)\right) \\ &= 0 + 0 \\ &= 0 \end{aligned}$$

as the (continuous) measure of single points is zero.

The set $N \cup M \cap \sigma_p(V)^{\mathrm{c}}$ must support m^{sc} as $N_1 \cap \sigma_p(V)^{\mathrm{c}}$ is a subset. Therefore

$$m^{sc}\left([N \cup M \cap \sigma_p(V)^{\mathrm{c}}]^{\mathrm{c}}\right) = 0.$$

This equals

$$\begin{aligned} m^{sc}\left([N \cup M]^{\mathrm{c}} \cup \sigma_p(V)\right) &= m^{sc}\left([N \cup M]^{\mathrm{c}}\right) + m^{sc}\left(\sigma_p(V)\right) \\ &= m^{sc}\left([N \cup M]^{\mathrm{c}}\right) \end{aligned}$$

so we conclude that the set $N \cup M$ supports the singular continuous part of the spectrum. □

Theorem 6.4 has shown us that V has an empty absolutely continuous component, and that the singular continuous component is supported by the set $N \cup M$, which is independent of λ. We know that N has measure zero, and Lemma 6.5 below shows us that M also has measure zero. This will allow us to apply Theorem 6.6 to show that the singular continuous spectrum of V is also empty. Thus, with both the absolutely continuous and singularly continuous spectra empty, we can conclude that V must have pure point spectrum.

Lemma 6.5 *Let $Q(z)$ be a trace class valued analytic function inside the complex unit circle, with $|z| < 1$. Then for a.e. θ*

$$\lim_{\epsilon \downarrow 0} Q\left(e^{i(\theta+i\epsilon)}\right) \equiv Q\left(e^{i(\theta+i0)}\right)$$

exists in Hilbert Schmidt norm.

Proof. We parallel the proof of de Branges theorem (see [34] and p. 149–150, [77]). Consider

$$\begin{aligned} &Q\left(e^{i(\theta+i\epsilon)}\right) + Q^*\left(e^{i(\theta+i\epsilon)}\right) \\ &\qquad = \int A^* \left\{ \frac{1}{1 - e^{-i(\theta'-\theta)}e^{-\epsilon}} + \frac{1}{1 - e^{i(\theta'-\theta)}e^{-\epsilon}} \right\} AE(d\theta') \\ &\qquad = \int A^* \left\{ \frac{2\left(1 - e^{-\epsilon}\cos(\theta'-\theta)\right)}{1 + e^{-2\epsilon} - 2e^{-\epsilon}\cos(\theta'-\theta)} \right\} AE(d\theta'). \end{aligned}$$

The factor within the curly braces is greater than zero for all θ', θ and thus we have

$$Q\left(e^{i(\theta+i\epsilon)}\right) + Q^*\left(e^{i(\theta+i\epsilon)}\right) \geq 0 \ \ \forall \epsilon \geq 0.$$

Therefore, following de Branges,

$$\begin{aligned} \left|\det\left(1 + Q\left(e^{i(\theta+i\epsilon)}\right)\right)\right|^2 &\geq \det\left(1 + Q^*\left(e^{i(\theta+i\epsilon)}\right) Q\left(e^{i(\theta+i\epsilon)}\right)\right) \\ &= \prod\left(1 + |\alpha_n|^2\right) \\ &\geq \begin{cases} \sum |\alpha_n|^2 = \|Q\left(e^{i(\theta+i\epsilon)}\right)\|^2_{H.S.} \\ 1. \end{cases} \end{aligned}$$

$\{\alpha_n\}$ are the eigenvalues of $Q\left(e^{i(\theta+i\epsilon)}\right)$. From these two bounds we obtain

$$\left\| \frac{Q\left(e^{i(\theta+i\epsilon)}\right)}{\det\left(1 + Q\left(e^{i(\theta+i\epsilon)}\right)\right)} \right\|_{H.S.} \leq 1 \text{ and } \left| \frac{1}{\det\left(1 + Q\left(e^{i(\theta+i\epsilon)}\right)\right)} \right| \leq 1.$$

The definition of an analytic operator (p. 189, [94]) implies the analyticity of the eigenvalues, and thus the operations of taking the determinant and the Hilbert Schmidt norm are analytic. Hence, both functions above are analytic and bounded within the complex unit circle ($\epsilon > 0$). Application of Fatou's theorem (p. 454, [36]) establishes the existence in the limit as $\epsilon \to 0$ and hence both functions exist on the boundary almost everywhere. Taking the quotient we establish the existence of $Q\left(e^{i(\theta+i0)}\right)$ in the Hilbert Schmidt norm. □

Let (Ω, μ) be a separable measure space, and

$$V(\lambda) = \int e^{-i\theta} E_\lambda(d\theta)$$

a measurable family of unitary operators on $\mathcal{H}$. We denote by

$$\mathbb{V} = \int e^{-i\theta} \mathbb{E}(d\theta)$$

the multiplication operator

$$(\mathbb{V}u)(\lambda) = V(\lambda)u(\lambda)$$

on $L^2(\Omega, \mu; \mathcal{H})$, where $u(\lambda) \in L^2(\Omega, \mu; \mathcal{H})$.

A vector $u(\lambda)$ is an element of $L^2(\Omega, \mu; \mathcal{H})$ if, for $u(\lambda) \in \mathcal{H}$,

$$\int_{-\infty}^{\infty} \|u(\lambda)\|^2 \ d\mu < \infty.$$

It is important to note the difference between $V(\lambda)$ acting on $\mathcal{H}$ and $\mathbb{V}$ acting on $L^2(\Omega, \mu; \mathcal{H})$. To obtain our goal of showing that for a.e. λ, $V(\lambda)$ has a pure point spectrum, we must show that $\mathbb{V}$ is absolutely continuous as a function of λ on the space $L^2(\Omega, \mu; \mathcal{H})$.

Theorem 6.6 is taken directly from [66]. The proof given is, apart from some small notational changes, identical to that in [66]. Due to a number of typographical errors however, I have reproduced the proof here for reference and clarity.

THEOREM 6.6 *Let $\mathbb{V}$ be absolutely continuous on $L^2(\Omega, \mu; \mathcal{H})$, and assume that there is a fixed set S of Lebesgue measure zero which supports the singular continuous spectrum of $V(\lambda)$ in the interval J for μ-a.e. λ. Then $V(\lambda)$ has no singular continuous spectrum in J for μ-a.e. λ.*

Proof. For fixed $x \in \mathcal{H}$, and any measurable subset Γ of Ω, let $u(\lambda) = \chi_\Gamma(\lambda)x$ be a vector in $L^2(\Omega, \mu; \mathcal{H})$. Then

$$\begin{aligned}\int_\Gamma |E_\lambda^{sc}[J]x|^2\,\mu(d\lambda) &\leq \int_\Gamma |E_\lambda[S]x|^2\,\mu(d\lambda)\\ &= \int |E_\lambda[S]u(\lambda)|^2\,\mu(d\lambda)\\ &= \int |\mathbb{E}[S]u(\lambda)|^2\,\mu(d\lambda)\\ &= \|\mathbb{E}[S]u(\lambda)\|^2 = 0.\end{aligned}$$

$\int_\Gamma |E_\lambda^{sc}[J]x|^2\,\mu(d\lambda) = 0$ implies that $|E_\lambda^{sc}[J]x|^2 = 0$ for μ-a.e. λ. Thus

$$E_\lambda^{sc}[J]x = 0$$

for every $x \in \mathcal{H}$. □

The application of Theorem 6.6 relies on finding a fixed set S of measure zero which supports the singularly continuous spectrum. $S = N \cup M$ is sufficient.

I have now established all the basic requirements for V to be pure point, given U pure point. They are now combined to produce the main theorem of the chapter. There is still quite a lot of manipulation to satisfy the condition $\mathbb{V}$ absolutely continuous on $L^2(\mathbb{R}; \mathcal{H})$ of Theorem 6.6, and this will be the focus for the remainder of Section 6.2 and Section 6.3.

THEOREM 6.7 *Let U and A satisfy the hypotheses of Theorem 6.4 and define for $\lambda \in \mathbb{R}$*

$$V(\lambda) = e^{i\lambda A^* A/\hbar} U.$$

Then $V(\lambda)$ is pure point in J for a.e. λ.

Proof. By Theorem 6.4, with $W = \lambda I$, $V(\lambda)$ has no absolutely continuous spectrum in J, and its singularly continuous spectrum is supported on the fixed set $S = N \cup M$. Application of Lemma 6.5 shows that S is of measure zero. If we can show that $\mathbb{V}$ is absolutely continuous on $L^2(\mathbb{R}; \mathcal{H})$ then Theorem 6.6 applies and shows that the singular continuous spectrum is empty. I prove the absolute continuity of $\mathbb{V}$ in the following sections.

As I have shown that both the absolutely continuous and singular continuous parts of the spectrum are empty, we conclude that $V(\lambda)$ is pure point for a.e. $\lambda \in \mathbb{R}$. □

To show that $\mathbb{V}$ is absolutely continuous, I apply a modified version of the Putnam–Kato theorem which is proved in Section 6.3. The unitary Putnam–Kato theorem is:

Theorem 6.11 *Let V be unitary, and D a self-adjoint bounded operator. If $C = V[V^*, D] \geq 0$, then V is absolutely continuous on $R(C^{1/2})$. Hence, if $R(C^{1/2})$ is cyclic for V, then V is absolutely continuous on $\mathcal{H}$.*

I apply this theorem on the space $L^2(\mathbb{R}; \mathcal{H})$. A naive application to obtain the desired result is as follows. I slightly change notation and explicitly include the λ dependence of W in the definition of V. If we choose $\mathbb{D} = -i(d/d\lambda)$, with

$V = e^{i\lambda A^*WA}U$, then

$$-i\frac{dV^*}{d\lambda} = -U^*A^*WAe^{-i\lambda A^*WA} = -V^*A^*WA,$$

so that for some $u \in L^2(\mathbb{R};\mathcal{H})$,

$$\begin{aligned}[\mathbb{V}^*, \mathbb{D}]u &= (\mathbb{V}^*\mathbb{D} - \mathbb{D}\mathbb{V}^*)u = -\mathbb{D}\mathbb{V}^*u \\ &= i\frac{d}{d\lambda}(\mathbb{V}^*u) = \mathbb{V}^*A^*WAu.\end{aligned}$$

Therefore,

$$\mathbb{C} = \mathbb{V}[\mathbb{V}^*, \mathbb{D}] = A^*WA.$$

With $W = I$, we obtain $\mathbb{C} = A^*A \geq 0$ and thus $R(\mathbb{C}^{1/2}) = R(A^*)$ (see the proof to (Theorem VI.9, [94])) is cyclic for V. Hence, $\mathbb{V}$ is absolutely continuous and all the requirements of Theorem 6.7 are satisfied.

The problem here is that $\mathbb{D}$ is not bounded, and boundedness of $\mathbb{D}$ is essential in the proof of the Putnam–Kato theorem. I use a similar technique as Howland [66] to overcome this issue.

As the norm of A^*A may be scaled arbitrarily, we can rewrite V, for real t, as

$$V(t) = e^{ictA^*A}U \tag{6.33}$$

for some real $c > 0$.

Proposition 6.8 *On $L^2(\mathbb{R};\mathcal{H})$, consider the unitary multiplication operator $\mathbb{V}$, defined by*

$$\mathbb{V}u(t) = V(t)u(t) = e^{ictA^*A}Uu(t)$$

and the bounded self-adjoint operator $\mathbb{D} = -\arctan(p/2)$, where $p = -id/dt$. Then $C = \mathbb{V}[\mathbb{V}^*, D]$ is positive definite, and $R\left(C^{1/2}\right)$ is cyclic for $\mathbb{V}$. Hence, the requirements of Theorem 6.7 are fully satisfied.

Proof. The operator $\mathbb{D}$ on $L^2(\mathbb{R};\mathcal{H})$ is convolution by the Fourier transform of $-\arctan(x/2)$ [66], which is $i\pi t^{-1}e^{-2|t|}$ ((3), p. 87, [41]). This is a singular (principal value) integral operator, because $\arctan(p/2)$ does not vanish at infinity. Thus, for $u(t) \in L^2(\mathbb{R};\mathcal{H})$,

$$\mathbb{D}u(t) = i\pi P \int_{-\infty}^{\infty} \frac{e^{-2|t-y|}}{t-y} u(y)\, dy$$

and

$$[\mathbb{V}^*, \mathbb{D}]u(t) = i\pi P \int_{-\infty}^{\infty} e^{-2|t-y|} \frac{V^*(t) - V^*(y)}{t-y} u(y)\, dy$$

so

$$\begin{aligned}\mathbb{C}u(t) &= \mathbb{V}[\mathbb{V}^*, \mathbb{D}]u(t) \\ &= i\pi P \int_{-\infty}^{\infty} e^{-2|t-y|} \frac{1 - V(t)V^*(y)}{t-y} u(y)\, dy.\end{aligned} \tag{6.34}$$

Inserting expression (6.33) for $V(t)$, we obtain

$$\begin{aligned}\mathbb{C}u(t) &= i\pi \int_{-\infty}^{\infty} e^{-2|t-y|} \frac{1 - e^{ic(t-y)A^*A}}{t-y} u(y)\, dy \\ &= i\pi \int_{-\infty}^{\infty} e^{-2|t-y|} \frac{1 - \cos\left(A^*Ac(t-y)\right) - i\sin\left(A^*Ac(t-y)\right)}{t-y} u(y)\, dy.\end{aligned} \tag{6.35}$$

Note that this is no longer a singular integral. To show that $\mathbb{C}$ is positive, we must show that

$$(u(t), \mathbb{C}u(t)) > 0 \;\; \forall u(t) \in L^2(\mathbb{R};\mathcal{H}).$$

Note that the inner product on $L^2(\mathbb{R};\mathcal{H})$ is given by

$$(u(t), u'(t)) = \int_{-\infty}^{\infty} u^*(t)u'(t)\, dt. \tag{6.36}$$

The operator A is now written in terms of its spectral components. Note that here λ decomposes A and bears no relation to the strength parameter used at other stages in this chapter. When required for clarity, I write $\int_\lambda$ to identify the integral over the variable λ,

$$A = \int \lambda E(d\lambda).$$

A general vector $u(t)$ may be written

$$u(t) = \int E(d\lambda)u(t).$$

Then

$$f(A)u(t) = \int f(\lambda)E(d\lambda)u(t)$$

which implies that we may rewrite (6.35) as

$$\begin{aligned}
\mathbb{C}u(t) &= i\pi \int_{-\infty}^{\infty} dy \int_\lambda e^{-2|t-y|} \frac{1 - e^{ic(t-y)|\lambda|^2}}{t-y} E(d\lambda)u(y) \\
&= \int_{-\infty}^{\infty} dy \int_\lambda \phi_\lambda(t-y)E(d\lambda)u(y) \\
&= \int_\lambda E(d\lambda)\mathcal{C}_\lambda(t)
\end{aligned}$$

where

$$\mathcal{C}_\lambda(t) = \int_{-\infty}^{\infty} dy\, \phi_\lambda(t-y)u(y)$$

and we have defined the new function

$$\phi_\lambda(t) = i\pi e^{-2|t|}t^{-1}\left(1 - e^{ict|\lambda|^2}\right).$$

By the convolution theorem, note that

$$\tilde{\mathcal{C}}_\lambda(\omega) = \tilde{\phi}_\lambda(\omega)\tilde{u}(\omega)$$

where the "˜" indicates Fourier transform.

Using this decomposition of $u(t)$ and Parseval's theorem, we can now easily write down $(u(t), \mathbb{C}u(t))$. I use $(x, y)_{\mathcal{H}}$ to indicate the inner product on the Hilbert

Space $\mathcal{H}$, reserving (x, y) for the inner product on $L^2(\mathbb{R}; \mathcal{H})$ as in (6.36).

$$
\begin{aligned}
(u(t), \mathbb{C}u(t)) &= \int_{-\infty}^{\infty} dt\ (u(t), \mathbb{C}u(t))_{\mathcal{H}} \\
&= \int_{-\infty}^{\infty} dt \left(u(t), \int_{\lambda} E(d\lambda)\mathcal{C}_{\lambda}(t) \right)_{\mathcal{H}} \\
&= \int_{-\infty}^{\infty} dt \left(u(t), \int_{\lambda} E(d\lambda) \int_{-\infty}^{\infty} dy\, \phi_{\lambda}(t-y)u(y) \right)_{\mathcal{H}} \\
&= \int_{-\infty}^{\infty} dt \left(u(t), \int_{\lambda} E(d\lambda) \int \frac{d\omega}{2\pi}\, e^{i\omega t}\tilde{\mathcal{C}}_{\lambda}(\omega) \right)_{\mathcal{H}} \\
&= \int_{\lambda} E(d\lambda) \int \frac{d\omega}{2\pi} \left(\tilde{u}(\omega), \tilde{\phi}_{\lambda}(\omega)\tilde{u}(\omega) \right)_{\mathcal{H}} \\
&= \int_{\lambda} E(d\lambda) \int \frac{d\omega}{2\pi}\ |\tilde{u}_{\lambda}(\omega)|^2\, \tilde{\phi}_{\lambda}(\omega).
\end{aligned}
$$

It is clear that if $\tilde{\phi}_{\lambda}(\omega)$ is positive for all λ then $\mathbb{C}$ will be positive.

In the following calculation we will find the need to bound $c|\lambda|^2$. The restriction $0 \leq c|\lambda|^2 \leq 1$ will be employed. I argue that as A^*A is a positive self-adjoint bounded operator we can restrict the integral over λ to ([98], p. 262, 273)

$$
A^*A = \int_{-\infty}^{\infty} |\lambda|^2 E(d\lambda) = \int_{m-0}^{M} |\lambda|^2 E(d\lambda) \tag{6.37}
$$

where M is the least upper bound and m the greatest lower bound of A^*A. The norm of A^*A is given by $\max(|m|, |M|)$. Thus, by setting

$$
c = \frac{1}{\|A^*A\|}
$$

then each $c|\lambda|^2$ is guaranteed to be less than unity.

Proceeding, the Fourier transform, $\tilde{\phi}_{\lambda}(\omega)$, of

$$
\phi_{\lambda}(t) = i\pi e^{-2|t|}t^{-1}\left[1 - \cos ct|\lambda|^2 - i \sin ct|\lambda|^2\right] \tag{6.38}
$$

is now calculated. Split (6.38) into two parts,

$$
\phi_{\lambda 1}(t) = i\pi e^{-2|t|}t^{-1}\left[1 - \cos ct|\lambda|^2\right], \tag{6.39}
$$

$$
\phi_{\lambda 2}(t) = \pi e^{-2|t|}t^{-1} \sin ct|\lambda|^2. \tag{6.40}
$$

The Fourier transform of (6.39) is

$$\begin{aligned}\tilde{\phi}_{\lambda 1}(\omega) &= i\pi \int_{-\infty}^{\infty} e^{-2|t|} t^{-1}(1 - \cos ct|\lambda|^2) e^{-i\omega t}\, dt \\ &= i\pi \left[\int_0^{\infty} e^{-2t} t^{-1}(1 - \cos ct|\lambda|^2) e^{-i\omega t}\, dt \right. \\ &\quad \left. + \int_0^{\infty} e^{-2t}(-t^{-1})(1 - \cos ct|\lambda|^2) e^{i\omega t}\, dt \right].\end{aligned}$$

Using ([41], p. 157, (59)), and setting $S = c|\lambda|^2/(2 + i\omega)$, we obtain

$$\tilde{\phi}_{\lambda 1}(\omega) = \frac{i\pi}{2} \log\left(\frac{1 + S^2}{1 + S^{*2}}\right).$$

The logarithm of a complex number can in general be written as

$$\log(z) = \log(|z|) + i\,\mathrm{Arg}\, z$$

so noting that $|(1 + S^2)/(1 + S^{*2})| = 1$, we see that

$$\begin{aligned}\tilde{\phi}_{\lambda 1}(\omega) &= -\frac{\pi}{2} \mathrm{Arg}\left(\frac{1 + S^2}{1 + S^{*2}}\right) \\ &= -\pi\, \mathrm{Arg}\left(1 + S^2\right).\end{aligned}$$

With $\kappa = c|\lambda|^2$, the real and imaginary parts of $1 + S^2$ are

$$\begin{aligned}\Re\left(1 + S^2\right) &= \frac{\left(4 + \omega^2\right)^2 + \kappa^2\left(4 - \omega^2\right)}{\left(4 + \omega^2\right)^2}, \\ \Im\left(1 + S^2\right) &= \frac{-4\kappa^2\omega}{\left(4 + \omega^2\right)^2}.\end{aligned}$$

With the restriction that $0 \le \kappa \le 1$, the real part is positive for all ω and thus $\mathrm{Arg}(z) = \arctan(\Im z/\Re z)$. Thus,

$$\tilde{\phi}_{\lambda 1}(\omega) = -\pi \arctan\left(\frac{\Im\left(1 + S^2\right)}{\Re\left(1 + S^2\right)}\right).$$

$\arctan(z)$ is the principal part of $\mathrm{Arctan}(z)$, with range $-\pi/2 < \arctan(z) < \pi/2$. The Fourier transform of (6.40) is similarly calculated, using ([41], p. 152, (16)), to be

$$\begin{aligned}\tilde{\phi}_{\lambda 2}(\omega) &= \pi\left[\arctan S + \arctan S^*\right] \\ &= \pi\left[\arctan\left(\frac{c|\lambda|^2}{2+i\omega}\right) + \arctan\left(\frac{c|\lambda|^2}{2-i\omega}\right)\right].\end{aligned}$$

Repeated application of the formula $\arctan(z_1)+\arctan(z_2) = \arctan(z_1+z_2/1-z_1z_2)$, valid when $z_1z_2 < 1$ (true for $0 \leq \kappa \leq 1$), yields[4]

$$\begin{aligned}\tilde{\phi}_{\lambda}(\omega) &= \tilde{\phi}_{\lambda 1}(\omega) + \tilde{\phi}_{\lambda 2}(\omega) \\ &= \pi\arctan\left(\frac{n(\omega, c|\lambda|^2)}{d(\omega, c|\lambda|^2)}\right), \end{aligned} \tag{6.41}$$

where

$$n(\omega,\kappa) = 4\kappa\left[\left(4+\omega^2\right)^2 + \kappa\omega\left(4+\omega^2\right) + \kappa^2\left(4-\omega^2\right) - \kappa^3\omega\right] \tag{6.42}$$

and

$$d(\omega,\kappa) = \left(4+\omega^2\right)^3 - 2\kappa^2\omega^2\left(4+\omega^2\right) - 16\kappa^3\omega - \kappa^4\left(4-\omega^2\right). \tag{6.43}$$

We can easily confirm that for $0 \leq \kappa \leq 1$, $n(\omega,\kappa)/d(\omega,\kappa)$ and hence $\tilde{\phi}_{\lambda}(\omega)$ is strictly positive by noting that there are four distinct regions of interest for ω, in which terms in n and d do not change sign. Table 6.1 shows these regions and the sign of each term in the region. Note that the global (positive and hence irrelevant) κ factor from (6.42) is dropped from the numerator for the following discussion.

[4]This result is not valid for values of κ larger than around 2, at which point the $\arctan$ addition formulas fail—this is a moot point however, as we may trivially restrict κ as already explained.

$n(\omega,\kappa) =$	$(4+\omega^2)^2$	$+\kappa\omega\,(4+\omega^2)^2$	$+\kappa^2\,(4-\omega^2)$	$-\kappa^3\omega$
$\omega < -2$	+ve	-ve	-ve	+ve
$-2 < \omega < 0$	+ve	-ve	+ve	+ve
$0 < \omega < 2$	+ve	+ve	+ve	-ve
$\omega > 2$	+ve	+ve	-ve	-ve

$d(\omega,\kappa) =$	$(4+\omega^2)^3$	$-2\kappa^2\omega^2\,(4+\omega^2)$	$-16\kappa^3\omega$	$-\kappa^4\,(4-\omega^2)$
$\omega < -2$	+ve	-ve	+ve	+ve
$-2 < \omega < 0$	+ve	-ve	+ve	-ve
$0 < \omega < 2$	+ve	-ve	-ve	-ve
$\omega > 2$	+ve	-ve	-ve	+ve

Table 6.1: Sign of each term in the numerator $n(\omega,\kappa)$ and the denominator $d(\omega,\kappa)$ of (6.41).

For each row in the table, we simply need to show that the terms add to produce a strictly positive number. First note that the first column for both the numerator and denominator is independent of κ. To show the positivity of each row, set all positive κ-dependent terms to zero and then take $\kappa = 1$ for the negative terms to maximise their contribution. Expanding out terms, it is then trivially seen in all cases that the first column ($(4+\omega^2)^2$ for the numerator and $(4+\omega^2)^3$ for the denominator) dominates. Thus, no row is negative and we conclude that $\tilde{\phi}_\lambda$ is positive definite.

We have established that the Fourier transform of ϕ_λ is positive definite for $c|\lambda|^2 \leq 1$. As a visual aid, Figure 6.1 shows $\tilde{\phi}_\lambda(\omega)$. The positivity for $c|\lambda|^2 \leq 1$ is clear.

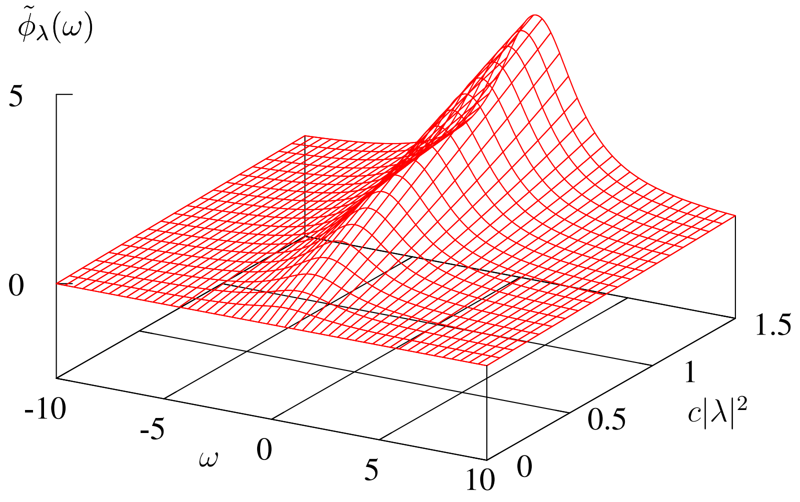

Figure 6.1: Plot of $\tilde{\phi}_\lambda(\omega) = \tilde{\phi}_{\lambda 1}(\omega) + \tilde{\phi}_{\lambda 2}(\omega)$, the Fourier transform of $\phi_\lambda(t) = i\pi e^{-2|t|}t^{-1}\left(1 - \cos(ct|\lambda|^2) - i\sin(ct|\lambda|^2)\right)$. $\tilde{\phi}_\lambda(\omega)$ is strictly positive for all ω when $c|\lambda|^2 \leq 1$.

Thus, $\mathbb{C}$ is strictly positive and $\mathbb{V}$ is absolutely continuous on $R(\mathbb{C}^{1/2})$. As A^*A is a factor of $1 - e^{ictA^*A}$ (i.e., A^*A is a factor of $\mathbb{C}$), $R(\mathbb{C}^{1/2}) = R(A^*)$. Noting that $R(A^*)$ is cyclic for U and hence cyclic for V, we conclude that $R(\mathbb{C}^{1/2})$ is cyclic for $\mathbb{V}$. Thus, $\mathbb{V}$ is absolutely continuous on $L^2(\mathbb{R};\mathcal{H})$. $\square$

I have now satisfied all the requirements of Theorem 6.7.

6.3 The unitary Putnam–Kato theorem

In this section, I will prove a modified version of the Putnam–Kato theorem, as used in the preceding section. The theorems and proofs follow a similar argument to that of Reed and Simon (Theorem XIII.28, p. 157, [96]) and are motivated by the stroboscopic nature of the kicked Hamiltonian.

DEFINITION 6.9 (V-SMOOTH) *Let V be a unitary operator. A is V-smooth if and only if for all $\phi \in \mathcal{H}$, $V(t)\phi \in D(A)$ for almost every $t \in \mathbb{R}$ and for some constant C,*

$$\sum_n \|AV^n\phi\|^2 \leq C\, \|\phi\|^2 \,.$$

THEOREM 6.10 *If A is V-smooth, then $\overline{R(A^*)} \subset \mathcal{H}_{ac}(V)$.*

Proof. Since $\mathcal{H}_{ac}(V)$ is closed, we need only show $R(A^*) \subset \mathcal{H}_{ac}(V)$. Let $\phi \in D(A^*)$, $\psi = A^*\phi$, and let $d\mu_\psi$ be the spectral measure for V associated with ψ. Define, for the period, T, in (6.1),

$$\mathcal{F}_n(T) = \frac{1}{\sqrt{2\pi}}\left(A^*\phi, [V(T)]^n\psi\right). \tag{6.44}$$

We calculate, dropping the T for clarity,

$$\begin{aligned}|\mathcal{F}_n| &= \frac{1}{\sqrt{2\pi}}\,|(\phi, AV^n\psi)| \\ &\leq \frac{1}{\sqrt{2\pi}}\,\|\phi\|\|AV^n\psi\| \,.\end{aligned}$$

Because A is V-smooth, we see that

$$\begin{aligned}\sum_n |\mathcal{F}_n|^2 &\leq \frac{1}{2\pi}\,\|\phi\|^2 \sum_n \|AV^n\psi\|^2 \\ &\leq \frac{C}{2\pi}\,\|\phi\|^2\|\psi\|^2 \\ &< \infty.\end{aligned}$$

Thus, $\mathcal{F}_n \in L^2(\mathbb{R})$. By the Riesz–Fischer theorem (4.26 Fourier Series, p. 96–7, [100]), $\mathcal{F}(\theta) = \frac{1}{\sqrt{2\pi}} \sum_n \mathcal{F}_n e^{-in\theta} \in L^2$.

The spectral resolution of $V[T]$ is

$$V[T] = \int_0^{2\pi} e^{i\theta}\, dE_T(\theta),$$

so

$$(V[T])^n = \int_0^{2\pi} e^{in\theta}\, dE_T(\theta).$$

Therefore, from (6.44) we obtain

$$\begin{aligned}\mathcal{F}_n &= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \left(A^*\phi, e^{in\theta}\, dE_T(\theta)\psi\right) \\ &= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{in\theta}\, (\psi, dE_T(\theta)\psi) \\ &= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{in\theta}\, d\mu_\psi(\theta).\end{aligned}$$

Using the inverse of the expression above for $\mathcal{F}(\theta)$ gives

$$\mathcal{F}_n = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{in\theta} \mathcal{F}(\theta)\, d\theta.$$

As we have just shown that $\mathcal{F}(\theta) \in L^2$, $d\mu_\psi(\theta) = \mathcal{F}(\theta) d\theta$ is absolutely continuous, which implies that $\psi \in R(A^*)$ is in $\mathcal{H}_{ac}(V)$ and so $\overline{R(A^*)} \subset \mathcal{H}_{ac}(V)$. □

THEOREM 6.11 (UNITARY PUTNAM–KATO THEOREM) *Let V be a unitary operator, and A a self-adjoint bounded operator. If $C = V[V^*, A] \geq 0$, then V is absolutely continuous on $R(C^{1/2})$. Hence, if $R(C^{1/2})$ is cyclic for V, then V is absolutely continuous.*

Proof. The discrete time evolution of an operator A is given by

$$\mathcal{F}_n = V^{-n} A V^n.$$

Calculate

$$\begin{aligned}\mathcal{F}_n - \mathcal{F}_{n-1} &= V^{-n}AV^n - V^{-(n-1)}AV^{(n-1)} \\ &= V^{-n}[AV - VA]V^{(n-1)} \\ &= V^{-n}V[V^{-1}A - AV^{-1}]VV^{n-1} \\ &= V^{-n}V[V^*, A]V^n \\ &\equiv G_n,\end{aligned}$$

so

$$\begin{aligned}\sum_{n=a}^{b}(\phi, G_n\phi) &= \sum_{n=a}^{b}\big(\phi, V^{-n}V[V^*, A]V^n\phi\big) \\ &= \sum_{n=a}^{b}(V^n\phi, V[V^*, A]V^n\phi) \\ &= \sum_{n=a}^{b}\Big(C^{\frac{1}{2}}V^n\phi, C^{\frac{1}{2}}V^n\phi\Big) \\ &= \sum_{n=a}^{b}\|C^{\frac{1}{2}}V^n\phi\|^2 ,\end{aligned}$$

where $C = V[V^*, A]$. We also have

$$\sum_{n=a}^{b}(\phi, G_n\phi) = \big(\phi, V^{-b}AV^b\phi\big) - \big(\phi, V^{-(a-1)}AV^{(a-1)}\phi\big) .$$

Taking the modulus and using the Schwartz inequality yields

$$\begin{aligned}\sum_{n=a}^{b}\|C^{\frac{1}{2}}V^n\phi\|^2 &\le 2\left|\big(\phi, V^{-b}AV^b\phi\big)\right| \\ &= 2\left|\big(V^b\phi, AV^b\phi\big)\right| \\ &\le 2\ \|A\|\|V^b\phi\|^2 \\ &= 2\ \|A\|\|\phi\|^2 \\ &< \infty\end{aligned}$$

and thus $C^{1/2}$ is V-smooth.

Finally, that V is absolutely continuous on $R(C^{1/2})$ follows directly from Theorem 6.10. □

6.4 Finite rank perturbations

Here, I utilise the results of Section 6.2 to show that perturbations of the form (6.5) lead to a pure point spectrum for the Floquet operator for a.e. perturbation strength λ.

I use directly the definition of *strongly H-finite* from Howland.

DEFINITION 6.12 (STRONGLY H-FINITE) *Let H be a self-adjoint operator on $\mathcal{H}$ with pure point spectrum, ϕ_n a complete orthonormal set of eigenvectors, and $H\phi_n = \alpha_n\phi_n$. A bounded operator $A : \mathcal{H} \to \mathcal{K}$ is strongly H-finite if and only if*

$$\sum_{n=1}^{\infty} |A\phi_n| < \infty. \tag{6.45}$$

If H is thought of as a diagonal matrix on l_2, i.e., $H = \sum_n \alpha_n |\phi_n\rangle\langle\phi_n|$, and A as an infinite matrix $\{a_{ij}\}$, i.e., $A = \sum_{m,n} a_{mn} |\phi_m\rangle\langle\phi_n|$, then (6.45) says

$$\sum_n \left[\sum_i |a_{in}|^2\right]^{\frac{1}{2}} < \infty. \tag{6.46}$$

For our purposes, we need to show that if A is strongly H-finite, then it is U-finite. To satisfy the assumption that Q_ϵ is trace class in Lemma 6.5 (and hence also compact in Theorem 6.4) we also need to show that A is trace class.

THEOREM 6.13 *If A is strongly H-finite, then given $U = e^{iTH/\hbar}$ for the period T in (6.1) and $H\phi_n = \alpha_n\phi_n$,*

(a) *A is trace class, and*

(b) *A is U-finite.*

Proof. (a) Simply consider

$$\mathrm{Tr}(A) = \sum_l \langle \phi_l \,|A|\, \phi_l \rangle = \sum_l a_{ll} \le \sum_l |a_{ll}| \,. \tag{6.47}$$

For each term in the sum (6.47) we trivially have

$$|a_{ll}| \le \sqrt{\sum_i |a_{il}|^2}$$

and thus (6.47) is finite so A is trace class.

(b) Noting that

$$U|\phi_n\rangle = e^{iTH/\hbar}|\phi_n\rangle = e^{iT\alpha_n/\hbar}|\phi_n\rangle$$

we calculate, by insertion of a complete set of states,

$$\begin{aligned}
&\sum_n \langle \phi_n | G_\epsilon(\theta; U, A) | \phi_n \rangle \\
&\quad = \sum_n \langle \phi_n | A \frac{1}{(1 - U^* e^{-i\theta_-})\,(1 - U e^{i\theta_+})} A^* | \phi_n \rangle \\
&\quad = \sum_{n,m} \langle \phi_n | A | \phi_m \rangle \langle \phi_m | \frac{1}{(1 - U^* e^{-i\theta_-})\,(1 - U e^{i\theta_+})} A^* | \phi_n \rangle \\
&\quad = \sum_{n,m} \frac{\langle \phi_n | A | \phi_m \rangle \langle \phi_m | A^* | \phi_n \rangle}{(1 - e^{-iT\alpha_m/\hbar} e^{-i\theta_-})\,(1 - e^{iT\alpha_m/\hbar} e^{i\theta_+})} \\
&\quad = \sum_{n,m} \frac{\langle \phi_m | A^* | \phi_n \rangle \langle \phi_n | A | \phi_m \rangle}{(1 - e^{-iT\alpha_m/\hbar} e^{-i\theta_-})\,(1 - e^{iT\alpha_m/\hbar} e^{i\theta_+})} \\
&\quad = \sum_m \frac{\langle \phi_m | A^* A | \phi_m \rangle}{|1 - e^{-\epsilon} e^{iT\alpha_m/\hbar} e^{i\theta}|^2} \\
&\quad = \sum_n \frac{\langle \phi_n | A^* A | \phi_n \rangle}{|1 - e^{-\epsilon} e^{iT\alpha_n/\hbar} e^{i\theta}|^2} .
\end{aligned}$$

The trace norm is then

$$\mathrm{Tr}\, G_\epsilon(\theta) = \sum_n \frac{|A\phi_n|^2}{|1 - e^{-\epsilon} e^{iT\alpha_n/\hbar} e^{i\theta}|^2} .$$

If this is bounded for $\epsilon = 0$, then it is trivially bounded for all $\epsilon > 0$. By (6.45) and a slightly modified version of (Theorem 3.1, [66]) this is finite a.e. for $\epsilon = 0$. Thus the trace norm of G_ϵ exists as $\epsilon \to 0$, which implies that the strong limit of G_ϵ exists and we conclude that A is U-finite. □

THEOREM 6.14 *Let U be a pure point unitary operator, and let $A_1, \ldots, A_N$ be strongly H-finite. Assume that the A_ks commute with each other. Then for a.e. $\lambda = (\lambda_1, \ldots, \lambda_N)$ in $\mathbb{R}^N$,*

$$V(\lambda) = e^{i\left(\sum_{k=1}^{N} \lambda_k A_k^* A_k\right)/\hbar} U$$

is pure point.

Proof. This is a trivial modification of (Theorem 4.3, [66]). Let

$$\mathcal{K} = \bigoplus_{k=1}^{N} \overline{R(A_k)}.$$

The elements of $\mathcal{K}$ are represented as column vectors. The operator $A : \mathcal{H} \to \mathcal{K}$ is defined, for $y \in \mathcal{H}$, by

$$Ay = \begin{bmatrix} A_1 y \\ \vdots \\ A_N y \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}$$

and therefore $A^* : \mathcal{K} \to \mathcal{H}$ is given by

$$A^* x = A_1^* x_1 + \cdots + A_N^* x_N.$$

Accordingly, $G_\epsilon(\theta) : \mathcal{K} \to \mathcal{K}$, the matrix equivalent of equation (6.9), is introduced,

$$\begin{aligned} &G_\epsilon(\theta; U, A) \\ &\quad = A\left[1 - U^* e^{-i\theta_-}\right]^{-1}\left[1 - U e^{i\theta_+}\right]^{-1} A^* \\ &\quad = \left\{A_i\left[1 - U^* e^{-i\theta_-}\right]^{-1}\left[1 - U e^{i\theta_+}\right]^{-1} A_j^*\right\}_{1 \le i,j \le N}. \end{aligned}$$

The diagonal terms are finite a.e. because each A_k is U-finite by Theorem 6.13. The off-diagonal terms are of the form $X_1^* X_2$, and so the Schwartz inequality,

$$|X_1^* X_2|^2 \leq \|X_1\|^2 \|X_2\|^2$$

ensures that they are finite a.e. too. Hence, A is U-finite as every term in the matrix $G_\epsilon(\theta; U, A)$ is a.e. finite as $\epsilon \to 0$.

The Hamiltonian may now be written as

$$H(\lambda) = H_0 + A^* W(\lambda) A \sum_{n=0}^{\infty} \delta(t - nT) \tag{6.48}$$

and the Floquet operator as

$$V(\lambda) = e^{iA^* W(\lambda) A/\hbar} U$$

where $W(\lambda) = \text{diag}\{\lambda_k\}$. In this form, the formalism of Section 6.2 is essentially fully regained, and we can proceed to apply Theorems 6.2, 6.4, 6.6 and 6.7.

To establish the absolute continuity of the multiplication operator $\mathbb{V}$ on the space $L^2(\mathbb{R}^N; \mathcal{H})$ we proceed as in Proposition 6.8. Write

$$V(t_1, \ldots, t_N) = e^{ic \sum_{k=1}^N t_k A_k^* A_k/\hbar} U,$$

define

$$D = -\sum_{k=1}^{N} \arctan(p_k/2),$$

where $p_k = -id/dt_k$, and compute

$$C = \mathbb{V}[\mathbb{V}^*, D] = \sum_{k=1}^{N} C_k \geq 0.$$

In obtaining C as a direct sum of the C_k, we have had to assume that the A_ks commute with each other. This complication comes when considering the term

$$V(t_1, \ldots, t_N) V^*(t_1, \ldots, t_{k-1}, y_k, t_{k+1}, \ldots, t_N)$$

in the equivalent of (6.34). To obtain the required form of $e^{ic(t_k-y_k)A_k^*A_k}$ we require that the A_ks commute.[5]

Moving on, each $C_k \geq 0$ is equivalent to C in Proposition 6.8 and hence positive. Finally, we must show that $R(C^{1/2})$ is cyclic for $\mathbb{V}$. This is no longer trivial as, for each k, while $R(C_k^{1/2}) = R(A_k^*)$, the range of A_k^* is not cyclic for U, hence $\mathbb{V}$. To proceed, first note that

$$R(A^*) = \bigcup_k R(A_k^*).$$

Now, as argued in Howland, we can assume that $R(A^*)$ is cyclic for U. To elaborate, define $\mathcal{M}(U, R(A^*))$ to be the smallest closed reducing subspace of $\mathcal{H}$ containing $R(A^*)$. If $R(A^*)$ is not cyclic for U, then $\mathcal{H} \ominus \mathcal{M}$ is not empty. However, as shown below, if $y \in \mathcal{H} \ominus \mathcal{M}$, then $A^*WAy = 0$, so in $\mathcal{H} \ominus \mathcal{M}$, $V(t) = U$ and is therefore pure point trivially. Thus, we can ignore the space $\mathcal{H} \ominus \mathcal{M}$ and restrict the discussion to $\mathcal{M}$—i.e., we may assume $R(A^*)$ cyclic for U.

The above relied upon showing that $A^*WAy = 0$ for $y \in \mathcal{H} \ominus \mathcal{M}$. I now prove this. If $y \in \mathcal{H} \ominus \mathcal{M}$ and $y' \in \mathcal{M}$, then

$$\langle y, y' \rangle = 0.$$

Given $y' \in \mathcal{M}$, there exists an $x \in \mathcal{K}$ such that $y' = A^*x$, so

$$\langle y, A^*x \rangle = 0.$$

That is

$$\langle Ay, x \rangle = 0.$$

This is true for all $x \in \mathcal{K}$. Suppose $y'' \in \mathcal{H}$. Then $WAy'' \in \mathcal{K}$ and so

$$\langle Ay, WAy'' \rangle = 0.$$

[5] This restriction is not required in Howland's self-adjoint work because the summation over k in the Hamiltonian (6.48) enters directly, rather than in the exponent of V.

That is

$$\langle A^* W A y, y'' \rangle = 0.$$

As this is true for any $y'' \in \mathcal{H}$, we conclude that $A^* W A y = 0$ on $\mathcal{H} \ominus \mathcal{M}$.

Thus, $R(A^*)$ (with A acting on $L^2(\mathbb{R}^{\mathbb{N}}; \mathcal{H})$) may be assumed cyclic for U, hence cyclic for $\mathbb{V}$.

I must finally show that $R(C^{1/2}) = R(A^*)$. We have

$$R(A^*) = \bigcup_k R(A_k^*) = \bigcup_k R(C_k^{1/2})$$

and

$$R(C) = \bigcup_k R(C_k).$$

As $R(A^*) = R(A^* A)$, $R(C^{1/2}) = R(C)$ and we have shown that $R(C^{1/2}) = R(A^*)$ as required. □

Finally, I wish to make the connection with my original aim—to show that Hamiltonians of the form

$$H(t) = H_0 + \sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k| \sum_{n=0}^{\infty} \delta(t - nT) \tag{6.49}$$

have a pure point quasi-energy spectrum.

THEOREM 6.15 *Let H_0 be pure point, and define our time-dependent Hamiltonian as in (6.49). If $\psi_1, \ldots, \psi_N \in l_1(H_0)$, then for a.e. $\lambda = (\lambda_1, \ldots, \lambda_N)$ in $\mathbb{R}^N$, the Floquet operator*

$$V = e^{i\left(\sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k|\right)/\hbar} U$$

has pure point spectrum.

Proof. This theorem is just a special case of Theorem 6.14 with the A_ks given by $|\psi_k\rangle\langle\psi_k|$. Noting (6.7), the A_ks clearly commute. As Howland shows, $|\psi\rangle\langle\psi|$

is strongly H-finite if and only if $\psi \in l_1(H_0)$. Thus Theorem 6.14 applies and the result follows. □

6.5 Discussion of results and potential applications

Of fundamental importance in showing that the quasi-energy spectrum remains pure point for a.e. perturbation strength λ was the fact that $\psi_k \in l_1(H_0)$. That is, if we write

$$|\psi_k\rangle = \sum_{n=0}^{\infty} (a_k)_n |\phi_n\rangle,$$

where the $|\phi_n\rangle$ are the basis states of H_0, then $\psi_k \in l_1(H_0)$ if and only if

$$\sum_{n=0}^{\infty} |(a_k)_n| < \infty.$$

If this requirement is dropped, and we only retain $\psi_k \in l_2(H_0)$, then (Theorem 3.1, [66]) fails and there is the possibility that $V(\lambda)$ will have a non-empty continuous spectrum. It was this fact that Milek and Seba [90] took advantage of in showing that the rank-1 kicked rotor could contain a singularly continuous spectral component under certain conditions on the ratio of the kicking frequency and the fundamental rotor frequency. They analysed two regimes of the perturbation. One where $\psi \in l_1(H_0)$, in which case the numerical results clearly showed pure point recurrent behaviour, and the other where $\psi \in l_2(H_0)$, but $\psi \notin l_1(H_0)$. In the second case, the authors further proved that the absolutely continuous part of the spectrum was empty,[6] and thus the system contained a singularly continuous spectral component. The numerical results reflected this, with a diffusive type energy growth being observed.

[6] It turns out that Milek and Seba actually made an assumption in obtaining this result which is as yet is unjustified. Chapter 7 investigates this in detail.

With the generalisation of Combescure's work here, namely Theorem 6.15, it is now possible to investigate the full class of rank-N kicked Hamiltonians. A sufficient requirement for recurrent behaviour has been shown to be $\psi_k \in l_1(H_0)$ and so I must turn my attention to perturbations where this requirement is no longer satisfied. This is the topic of Chapter 7.

6.6 Summary

I have shown, in a rigorous and general fashion, that the spectrum of the Floquet operator remains pure point for perturbations which are constructed from projection operators that are in turn built from Hilbert space vectors which are elements of $l_1(H_0)$. In simple terms, with the Hamiltonian perturbation $W = |\psi\rangle\langle\psi|$, one requires

$$\sum_n \left|W^{1/2}\phi_n\right| < \infty$$

for the Floquet operator to have a pure point spectrum for almost every perturbation strength.

As alluded to in Section 6.5, to investigate systems that may display chaotic behaviour I would like to relax, in a controlled manner, the conditions that lead to a pure point spectrum for V. The emergence of a continuous spectrum is a vital ingredient in making further progress. Chapter 7 investigates this question.

CHAPTER 7

A GENERALISATION OF THE WORK OF COMBESCURE AND MILEK & SEBA

Contents

This chapter extends the results of Combescure [28] in a number of ways. Firstly, as an alternative to the work just presented in Chapter 6 I directly extend Combescure's result on rank-1 perturbations to rank-N perturbations—pleasingly, the same results as in Chapter 6 are obtained. I will then move on to the important question of the emergence of a continuous spectral component of the Floquet operator. I extend all of the results of Combescure and also those of Milek and Seba [90] to rank-N perturbations.

The investigations lead, in a natural way, to a conjecture presented by Combescure [28] concerning the dependence of her results on the particular H_0 eigenvalue sequence. The analysis herein leads to a number-theoretic conjecture that has stood for over fifty years [112][1] on the estimation of finite exponential sums. Work already done in this area [15] will be examined in detail.

In examining the work of Milek and Seba, I highlight a number of misconceptions and rectify them. Worryingly though, their work is not in fact fully justified—a point so far missed in the literature. The resolution is directly linked to the number-theoretic investigations just mentioned.

[1] The reference is to the 1954 English translation of Vinogradov's original work, published in 1947. The work in Vinogradov's 1947 monograph incorporates results from a series of papers and a first monograph from 1937. It is unknown (to me) when the conjecture I refer to was first presented, but it was at least fifty years ago.

7.1 Outline and summary of results

In this chapter, I consider Hamiltonians of the form

$$H(t) = H_0 + \left(\sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k| \right) \sum_{n=0}^{\infty} \delta(t - nT) \tag{7.1}$$

where $\lambda_k \in \mathbb{R}$ and each vector $|\psi_k\rangle$ is a linear combination of the H_0 basis states, $|\phi_n\rangle$. See Section 6.1 for the definitions and properties of these objects.

As already discussed, the basic result is that if every $|\psi_k\rangle \in l_1(H_0)$ the spectrum will remain pure point for almost every set of perturbation strengths λ_k. If this condition is dropped for any one of the $|\psi_k\rangle$ then $V_{\lambda_1,\ldots,\lambda_N}$ is no longer pure point. On the subspace $\mathcal{H}_k$, the space for which $|\psi_k\rangle$ is a cyclic vector for the operator U, the spectrum is purely continuous.

The other key result of this chapter concerns a number-theoretic conjecture stated by Vinogradov [112]. For Milek and Seba's work to be properly justified, a sufficient condition is for Vinogradov's conjecture to be true. This observation is linked to the conjecture put forward by Combescure [28] and partially addressed by Bourget [15].

In Section 7.2 I extend Combescure's rank-1 theorem on the pure point spectral nature of V to the rank-N case. In Section 7.3 I then show the existence of a continuous spectrum for the case where H_0 is the harmonic oscillator and the perturbation is rank-N. In Section 7.4 I investigate Combescure's conjecture, the partial answer provided by Bourget and the link to number theory and Vinogradov's conjecture. Finally, in Section 7.5, I extend Milek and Seba's work to the rank-N case. A number of conceptual and mathematical errors are firstly highlighted and then resolved.

7.2 A rank-N generalisation of Combescure's first theorem

Consider the measures

$$m_{k,\lambda_k} = \langle\psi_k|E_{\lambda_k}(S)|\psi_k\rangle.$$

Each $|\psi_k\rangle$ admits a cyclic subspace of $\mathcal{H}$, $\mathcal{H}_k$. As argued in the later part of the proof of Theorem 6.14, on the space $\mathcal{H} \ominus \left(\bigoplus_{k=1}^{N} \mathcal{H}_k\right)$, the perturbation

$$\sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k|$$

is null and thus $V = U$ is trivially pure point. Henceforth, we may safely restrict the proof to the subspace $\bigoplus_{k=1}^{N} \mathcal{H}_k$ for which the vectors $|\psi_k\rangle$ form a cyclic set.

Directly following Combescure, the measure for a point $x \in [0, 2\pi)$ for the operator V acting on the state $|\psi_k\rangle$ is given by

$$m_{k,\lambda_k}(\{x\}) = \frac{-4(1+\mu_k)}{\mu_k^2} B_k(x), \tag{7.2}$$

where

$$\mu_k = e^{i\lambda_k/\hbar} - 1$$

and

$$B_k(x) = \left[\int_0^{2\pi} dm_{k,\lambda_k=0}(\theta)\ \left(\sin^2\left[(x-\theta)/2\right]\right)^{-1}\right]^{-1}.$$

This result is the essence of Lemma 1 in Combescure's work. When H_0 is pure point, it is a trivial calculation to show that

$$B_k^{-1}(x) = \sum_{n=0}^{\infty} \frac{|(a_k)_n|^2}{\sin^2\left[(x-\theta_n)/2\right]}. \tag{7.3}$$

Corollary 2 in Combescure's work is replaced with the following.

THEOREM 7.1 *Assume H_0 is pure point, with $\{\phi_n\}_{n\in\mathbb{N}}$ and $\{\alpha_n\}_{n\in\mathbb{N}}$ as eigenstates and eigenvalues. Let each*

$$\psi_k = \sum_{n=0}^{\infty}(a_k)_n\phi_n$$

be cyclic for H_0 (hence, cyclic for U and V) on $\mathcal{H}_k$ and $\langle\psi_k|\psi_l\rangle = \delta_{kl}$. Then e^{ix} belongs to the point spectrum of $V_{\lambda_1,\ldots,\lambda_N}$ if and only if

$$\prod_{k=1}^{N} B_k^{-1}(x) < \infty,$$

where

$$\theta_n = 2\pi\{\alpha_n/2\pi\hbar\},$$

$\{z\}$ being the fractional part of z.

Proof. (7.1) The proof follows that in Combescure. By the cyclicity of each $|\psi_k\rangle$ on $\mathcal{H}_k$ and the argument in Theorem 6.14, e^{ix} is an eigenvalue of $V_{\lambda_1,\ldots,\lambda_N}$ if and only if *every* $m_{k,\lambda_k}(\{\theta\}) \neq 0$ at $\theta = x$. As already mentioned, using

$$dm_{k,\lambda_k=0} = \sum_{n=0}^{\infty}|(a_k)_n|^2\delta(\theta-\theta_n)d\theta$$

we obtain, for each k,

$$B_k^{-1}(x) = \sum_{n=0}^{\infty}\frac{|(a_k)_n|^2}{\sin^2[(x-\theta_n)/2]}.$$

Now consider the eigenvalue e^{ix}. If it were to be that for some k, $m_{k,\lambda_k}(\{x\}) = 0$, then we would have found a vector, namely $|\psi_k\rangle$, such that $V|\psi_k\rangle$ was continuous. We have in fact found that the whole subspace $\mathcal{H}_k$ is continuous. Thus, for V to be pure point, every $m_{k,\lambda_k}(\{\theta\}) \neq 0$. Thus, we are lead to consider the requirement

$$\prod_{k=1}^{N} B_k^{-1}(x) < \infty.$$

□

As in Combescure, the relationship

$$\sum_{n=0}^{\infty} |(a_k)_n|^2 \operatorname{cotg}\left(\frac{x-\theta_n}{2}\right) = \operatorname{cotg}\frac{\lambda_k}{2\hbar} \tag{7.4}$$

also holds for each k. To show (7.4), consider each k separately. The proof is the same as for the rank-1 case. See [28]. Points to consider are that each projection operator in the rank-N projection is normalised and hence for every k we have

$$\sum_{n=0}^{N} |(a_k)_n|^2 = 1.$$

In order to complete the generalisation of Combescure's first theorem, we require, just as in Combescure, two additional Lemmas.

Lemma 7.2 *If* $\sum_{n=0}^{\infty} |(a_k)_n| < \infty$*, then* $B_k^{-1}(x) < \infty$ *for almost every* $x \in \mathbb{R}$.

For each $k \in 1, \ldots, N$ the proof is identical to that in Combescure.

Lemma 7.3 *The following two statements are equivalent.*

(a) *For almost every* $(\lambda_1, \ldots, \lambda_N)$*,* $V_{\lambda_1,\ldots,\lambda_N}$ *has only a point spectrum.*

(b) *For every* $k \in \{1, \ldots, N\}$ *and for almost every* x*,* $B_k(x) \neq 0$.

The proof is again virtually identical to Combescure's proof. For each k, the continuous part of the spectrum is supported outside the set $E_k = \{x \in [0, 2\pi) : B_k(x) \neq 0\}$ and, for $\lambda_k \neq 0$, the point part of dm_{k,λ_k} is supported by the set E_k. Thus, for $V_{\lambda_1,\ldots,\lambda_N}$ to be pure point for almost every $\lambda_1, \ldots, \lambda_N$ and for every k, we require

$$m_{k,\lambda_k}([0, 2\pi) \setminus E_k) = 0.$$

This in turn implies that for every k

$$\int_0^{2\pi} d\lambda'_k \, h(\lambda'_k) m_{k,\lambda_k}([0, 2\pi) \setminus E_k) = 0,$$

where $\lambda'_k = \lambda_k/\hbar$ and

$$h(\lambda) = 2\Re \frac{1}{1 - ce^{i\lambda}}$$

for some $|c| < 1$.

Combescure's Lemma 5 trivially applies for each k. Thus, I have generalised Combescure's work to obtain the result that the Floquet operator for the rank-N perturbed Hamiltonian has a pure point spectrum. As already mentioned, the result matches that obtained in Chapter 6.

7.3 A rank-N generalisation of Combescure's second theorem

Having shown that the Floquet operator remains pure point for perturbations constructed from the vectors $|\psi_k\rangle \in l_1(H_0)$, Combescure relaxes this condition to allow for the emergence of a continuous spectral component of the Floquet operator. This result is easily generalised to the rank-N case. The key point is that Combescure's technique applies independently for each k. I do not discuss the details of the rank-1 proof here at all, delaying an analysis to Section 7.4 where I will have the opportunity to generalise the results still further. Here, I simply provide the argument for why each k may be treated independently. Before proceeding, some subtleties of what Combescure actually shows are highlighted. They are seemingly overlooked by some in the literature (e.g., [90]).

The cyclicity requirement was essential in the proof that the Floquet operator spectrum was pure point. Here, we can happily ignore the cyclicity conditions, as our only goal is to establish the existence of a state in the continuous subspace $\mathcal{H}_{\text{cont}}$. We need not try and ensure the result obtained by considering $\langle\psi|E(S)|\psi\rangle$ is applicable to all other vectors in $\mathcal{H}$—the very idea is ill-formed as the perturbation is null on a subset of $\mathcal{H}$ and thus there is always part of $\mathcal{H}$ where V has a discrete spectrum. Milek and Seba seem to have missed this point, restating Combescure's theorem in a way that implies that all ψ are in $\mathcal{H}_{\text{cont}}$.

If

$$\langle \psi_k | E(\{x\}) | \psi_k \rangle = 0$$

then $\mathcal{H}_{ac}$ contains at least the state $|\psi_k\rangle$. The point to be mindful of is that this does not allow one to conclude that the Hilbert space for the operator V has $\mathcal{H}_{pp} = \emptyset$. It is this error that Milek and Seba [90] have made. To draw that conclusion would require an argument to show that a cyclic vector does in fact exist for V. This does not seem possible in the general context here.

Combescure's proof (Lemma 6 in [28]) that $\sigma_{\text{cont}}(V) \neq \emptyset$ is based on showing that $B^{-1}(x) \to \infty$ (equation (7.3)). As the spectral measure of a single point x is proportional to $B(x)$ (equation (7.2)), if $B^{-1}(x) \to \infty$, then the contribution of the single point is zero. That is, e^{ix} is in the continuous spectrum of the Floquet operator. Combescure argues (see Section 7.4 for details) that

$$B^{-1}(x) \geq \#S(x)$$

where $\#S(x)$ is the number of elements of a particular set S. She then shows (the bulk of the proof) that $\#S(x) \to \infty$ and thus $B^{-1}(x) \to \infty$. I generalise the result in a straightforward manner.

THEOREM 7.4 *Assume $\alpha_n = n\hbar\omega$ with ω irrational. If $|\psi_k\rangle \notin l_1(H_0)$ for at least one $k \in 1, \ldots, N$, then $\sigma_{cont}(V) \neq \emptyset$.*

Proof. (7.4) Following the same argument as for the rank-1 case, we take

$$|(a_k)_n| = n^{-\gamma} 2\pi$$

for the state $|\psi_k\rangle$, in such a way that the condition $\langle \psi_k | \psi_l \rangle = \delta_{kl}$ is preserved.

With this construction, Combescure's proof that the number of elements in $S(x)$ is infinite applies to each subsequence $S_k(x)$. The number of elements,

$\#S_k(x)$, in each sub-sequence for which $|\psi_k\rangle \notin l_1(H_0)$, is infinite. The Floquet operator for the rank-N perturbed harmonic oscillator obtains a continuous spectral component. □

7.3.1 Discussion

It must be noted that the proof presented by Combescure (Lemma 6, [28]) is only valid for the eigenvalue spectrum,

$$\alpha_n = n\hbar\omega$$

of the harmonic oscillator. Combescure does however conjecture that the argument will be valid for more general eigenvalue spectra, including the rotor,

$$\alpha_n \propto n^2.$$

For Milek and Seba's numerical work (using the rotor) to be based on valid mathematical arguments, a proof of this conjecture is required. Currently, no such proof exists. In Section 7.4 I show that if a conjecture from number theory on the estimation of exponential sums is true, then Milek and Seba's work can be justified. The rank-N generalisation is straightforward. Considering the number theory conjecture has stood for over fifty years, it seems we may have to wait quite some time for a proof.

For more general eigenvalue spectra (loosely $\alpha_n \propto n^j$) the situation is significantly better. For $j \geq 3$ Bourget [15] has made significant progress. A continuous component of the Floquet operator exists for certain constructions of $|\psi\rangle$. The conditions are complicated and more restrictive than the $|\psi\rangle \notin l_1(H_0)$ condition for the harmonic oscillator. The result is easily extended to the rank-N case due to the independence of each k as already discussed. Utilising the same number-theoretic conjecture as in the $j = 2$ case will also allow for improvements to the work of Bourget. See Section 7.4.

Returning to the harmonic oscillator case, by applying Theorem 7.4 we may conclude that for each $|\psi_k\rangle \notin l_1(H_0)$, $\mathcal{H}_k$ is purely continuous. Thus, by dropping the l_1 condition for all $|\psi_k\rangle$, I have shown that V is purely continuous on the subspace of $\mathcal{H}$ where the perturbation is non-zero. On the subspace of $\mathcal{H}$ where the perturbation is zero, $V = U$ trivially and thus that portion of the Hilbert space remains pure point.

7.4 Combescure's conjecture and number theory

Combescure makes a remark (Remark c., [28]) that she believes Theorem 7.4 (Lemma 6, Combescure [28]) is generalisable to include systems other than the harmonic oscillator. Explicitly, she conjectures that Hamiltonians, H_0, with eigenvalues, α_n, of the form

$$\alpha_n = \hbar \sum_{j=0}^{p} \beta_j n^j \tag{7.5}$$

with $\beta_j T/2\pi$ Diophantine for some $j : 1 \leq j \leq p$ will have the vector ψ in the continuous spectral subspace of V_λ.

At an intuitive level, one would expect this to be true. The precise nature of the eigenvalue spectra (proportional to n or a polynomial in n) should not make a significant difference. Milek [89] argues that Combescure's work can be used in the n^2 case based on evidence from some numerical work that shows that the sequences obtained are "almost random"—however, the argument is not entirely convincing to me. The cited numerical work of Casati *et. al.* [20] discusses the existence of correlations in the energy levels, rather than the lack of correlations. While the deviations from a Poisson distribution look small to the naked eye, Casati *et. al.* [20] find deviations from the expected Poisson distribution of up to

17 standard deviations. The energy levels are correlated—it is arguable that they are not characterisable as "almost random" as Milek asserts.

I began to explore the possibility of developing a proof to the conjecture. A few interesting results have come from this investigation and will be presented here. While doing this work, I was unaware that in late 2002, Bourget [15] produced a proof of a slightly modified conjecture for all but the $p = 2$ case in (7.5). The techniques used by Bourget are the same as those followed in my work. I will analyse Bourget's work, and highlight the key breakthrough made. I also provide a modified argument to obtain the proof which is, I believe, significantly easier to follow. Importantly, it also covers the $p = 2$ case missed by Bourget due to technical difficulties. However, it comes at the expense of relying upon a (quite reasonable) conjecture. I do not claim that what is presented is adequate on its own, but it does play a complementary role in understanding, or perhaps appreciating, Bourget's proof. The reliance on the conjecture simply removes the need for much of the technical wizardry in Bourget's proof. Use of the conjecture also strengthens the work. The work also indicates, or highlights, that Combescure's conjecture is solved by a number-theoretic conjecture that has stood for over fifty years. What seems a perfectly reasonable conjecture on physical grounds is shown to be directly related to an abstract mathematical conjecture.

In what follows, I will rely heavily upon the lemmas and theorems in Chapter 2 of [84]. I also use some results on Weyl sums from [112]. Of key importance is an understanding of Combescure's proof of her Lemma 6 on the emergence of a continuous spectrum for the kicked harmonic oscillator. This will be discussed at the appropriate time in this section.

7.4.1 Number theory

To investigate Combescure's conjecture we require two concepts from number theory—the classification of irrational numbers and the *discrepancy* of a sequence. I first introduce the concepts and define the relevant ideas. I then proceed to analyse the conjecture and the proof provided by Bourget. As the discussion progresses, the new work that I have done will be presented.

For any number β, define

- $[\beta]$, the integer part of β,
- $\{\beta\}$, the fractional part of β, and
- $\langle\beta\rangle = \min(\{\beta\}, 1 - \{\beta\})$.

$\langle\beta\rangle$ is simply the "distance to the nearest integer". Definition 7.5 is taken directly from Kuipers and Niederreiter (Definition 3.4, p. 121, [84]).

DEFINITION 7.5 *Let η be a positive real number or infinity. The irrational, β, is of type η if η is the supremum of all τ for which*

$$\underline{\lim}_{n\to\infty}\, q^{\tau}\langle q\beta\rangle = 0, \tag{7.6}$$

where q runs through the positive integers.

The idea behind this definition can be seen by considering *rational* $\beta = p/q'$ for integers p and q'. Run through the positive integers q. At $q = q'$, $\langle q\beta\rangle = 0$, and so there is no supremum η for τ in (7.6). In effect, $\eta \to \infty$. For irrational β, $\langle q\beta\rangle$ is never equal to zero but will approach zero. If the approach is very slow, then a small τ is enough to prevent (7.6) from approaching zero. $\langle q\beta\rangle$ approaching zero slowly is, in a sense, indicative of β being badly approximated by rational numbers. Even for very large q', p/q' remains a poor approximation to β. Thus, the smaller η, the stronger the irrationality of β. This is reasonable in the sense that rational βs act like numbers with $\eta \to \infty$. As stated in [84], all numbers β have type $\eta \geq 1$.

I now define the discrepancy of a sequence—a measure of the non-uniformity of the sequence. Consider a sequence of numbers[2] x_n in $[0, 1)$,

$$\omega = (x_n)_{n \in \mathbb{N}} \text{ with } x_n \in [0, 1).$$

For $0 \leq a < b \leq 1$ and positive integer N, $A([a, b), N)$ counts the number of terms of the sequence (up to x_N) contained in the interval $[a, b)$,

$$A([a, b), N) = \#\{n \leq N : x_n \in [a, b)\}.$$

DEFINITION 7.6 *The discrepancy D_N of the sequence ω is*

$$D_N(\omega) = \sup_{0 \leq a < b \leq 1} \left| \frac{A([a, b), N)}{N} - (b - a) \right|. \tag{7.7}$$

If the sequence ω is uniformly distributed in $[0, 1)$ then $D_N \to 0$ as $N \to \infty$. In this case, every interval $[a, b]$ in $[0, 1)$ gets its "fair share" of terms from the sequence ω.

Estimating the discrepancy of a sequence will turn out to be vital in the analysis of Combescure's work. The sequence of interest is basically the eigenvalue sequence for H_0, but I will discuss this in greater detail later.

The starting point for the estimations that we require is (equation (2.42), Chapter 2, [84]). This is a famous result obtained by Erdös and Turán. It states that

$$D_N \leq C \left(\frac{1}{m} + \sum_{h=1}^{m} \frac{1}{h} \left| \frac{1}{N} \sum_{n=1}^{N} e^{2\pi i h x_n} \right| \right) \tag{7.8}$$

[2]Equivalently, consider any sequence x_n and consider the discrepancy of the sequence modulo 1.

for any real numbers $x_1, \dots, x_N$ and any positive integer m. The sum

$$S = \sum_{n=1}^{N} e^{2\pi i h x_n}$$

is an example of a class of exponential sums known as *Weyl sums*, reflecting the pioneering work of Weyl on providing estimations for them. Vinogradov [112] improved on some of the estimations of Weyl. Weyl and Vinogradov's results concern the modulus of the sum, $|S|$, and characterise it as

$$|S| \leq \gamma N,$$

where N is the number of terms in the sum and γ tends to zero as $N \to \infty$. The subtle behaviour of γ is linked to the rational/irrational nature of the terms in the sequence.

I will use some basic results from the introductory chapter of [112]. In general, write

$$S = \sum_{n=1}^{N} \exp\left(2\pi i F(n)\right)$$

for some function $F(n)$. The application here is when

$$F(n) = \beta n^j.$$

For β rational (*not* the case I will be interested in) L. K. Hau proved that $|S|$ was of order

$$N^{1-(1/j)+\epsilon}$$

(p. 3, [112]) and that this estimate could not be much improved. Here, I am interested in the case where β is irrational. Estimations are much more difficult, and form the major aspect of the work by Vinogradov. The estimations depend upon making a rational approximation to β and are complicated functions of N and j. Very loosely, he obtains results like

$$|S| = O(N^{1-\rho'})$$

where

$$\rho' = \frac{1}{3(j-1)^2 \log 12j(j-1)}. \tag{7.9}$$

Vinogradov states

> It is a plausible conjecture that the estimate in (7.9) holds with ρ' replaced be $1/j - \epsilon \ldots$ A proof or disproof of this conjecture would be very desirable.

With the dual aim of extending Bourget's proof to the $p = 2$ case (the rotor considered by Milek and Seba) and "simplifying" Bourget's proof, I state this conjecture formally.

CONJECTURE 7.7 *Consider the sum*

$$S = \sum_{n=1}^{N} \exp 2\pi i n^j \beta_j.$$

For all N greater than some critical value,

$$|S| \leq cN^{1-(1/j)+\epsilon}$$

for all $\epsilon > 0$ and some constant $c \in \mathbb{R}$.

I do not attempt to prove Conjecture 7.7. Given the lengths gone to by Vinogradov to obtain the results presented above, it seems rather unlikely that a proof or disproof will be found any time soon.[3]

[3] Incremental improvements on the estimations presented by Vinogradov in [112] have been made over time. While Bourget [15] makes use of these improved results, the conjecture itself remains unproven which is the only result of any consequence in this discussion.

7.4.2 New results on discrepancy—upper and lower bounds

Armed with the estimations on Weyl sums, I now proceed to derive both upper and lower bounds on the discrepancy for sequences of the type

$$\omega_j = (n^j \beta)$$

for β of any type $\eta \geq 1$. It must be remembered that the upper bound obtained is contingent upon Conjecture 7.7. The lower bound obtained is not dependent upon any unproved conjectures. The result obtained highlights the "best possible" nature of the conjectured upper bound.

Firstly, (Lemma 3.2, p. 122, [84]) is generalised to arbitrary j.

LEMMA 7.8 *The discrepancy $D_N(\omega_j)$ of $\omega_j = (n^j \beta)$ satisfies*

$$D_N(\omega_j) \leq C \left(\frac{1}{m} + N^{1-(1/j)+\epsilon} c' \sum_{h=1}^{m} \frac{1}{h \langle h\beta \rangle} \right)$$

for any positive integer m and $\epsilon > 0$, where C and c' are absolute constants.

Proof. (7.8) Consider equation (7.8). It is applicable to the first N terms of the sequence ω_j. We have

$$D_N(\omega_j) \leq C \left(\frac{1}{m} + \frac{1}{N} \sum_{h=1}^{m} \frac{1}{h} \left| \sum_{n=1}^{N} e^{2\pi i h n^j \beta} \right| \right) \tag{7.10}$$

for any positive integer m. Consider the sum over n,

$$\left| \sum_{n=1}^{N} e^{2\pi i h n^j \beta} \right| .$$

Conjecture 7.7 allows this sum to be bounded by

$$c N^{1-(1/j)+\epsilon}.$$

We are free to write

$$c = \frac{c'}{|\sin \pi h \beta|}$$

as $\sin \pi h\beta$ is just some positive real number. Substituting this result into (7.10) gives

$$D_N(\omega_j) \leq C\left(\frac{1}{m} + N^{-(1/j)+\epsilon}c' \sum_{h=1}^{m} \frac{1}{h}\frac{1}{|\sin \pi h\beta|}\right).$$

Now following the argument at the end of (Lemma 3.2, [84]) the desired result is obtained. □

I now give the generalisation of (Theorem 3.2, [84]). It provides the "best" upper bound one could hope for when estimating the discrepancy of the sequence $\omega_j = (n^j\beta)$. Again, remember that the proof relies on Conjecture 7.7.

THEOREM 7.9 *Assume Conjecture 7.7 is true. Let β be of finite type η. Let j be a positive integer $j \geq 1$. Then, for every $\epsilon > 0$, the discrepancy $D_N(\omega_j)$ of $\omega_j = (n^j\beta)$ satisfies*

$$D_N(\omega_j) = O\left(N^{-(1/\eta j)+\epsilon}\right).$$

Proof. (7.9) Let $\epsilon > 0$ be fixed. By (Lemma 3.1 and Lemma 3.3, p. 121–3, [84]),

$$\sum_{h=1}^{m} \frac{1}{h\langle h\beta\rangle} = O\left(m^{\eta-1+\epsilon'}\right)$$

for a fixed $\epsilon' > 0$. Combining this with Lemma 7.8 gives

$$D_N(\omega_j) \leq C\left(\frac{1}{m} + N^{-(1/j)+\epsilon''}m^{\eta-1+\epsilon'}\right)$$

for all $m \geq 1$. Now choose $m = \left[N^{1/\eta j}\right]$. We obtain

$$\begin{aligned} D_N(\omega_j) &\leq C\left(N^{-(1/\eta j)} + N^{-(1/j)+\epsilon''+(1/j)-(1/\eta j)+\epsilon'/\eta j}\right) \\ &= O\left(N^{-(1/\eta j)+\epsilon}\right) \end{aligned}$$

where $\epsilon = \epsilon'' + \epsilon'/\eta j$. □

Theorem 7.9 is, in a sense, optimal. For functions f, g, define $f = \Omega(g)$ if $f/g \nrightarrow 0$.

THEOREM 7.10 *Let β be of finite type η. Let j be a positive integer $j \geq 1$. Then, for every $\epsilon > 0$, the discrepancy $D_N(\omega_j)$ of $\omega_j = (n^j\beta)$ satisfies*

$$D_N(\omega_j) = \Omega\left(N^{-(1/\eta j)-\epsilon}\right).$$

Proof. (7.10) Let $\epsilon > 0$ be fixed. For any given $\epsilon' > 0$, there exists $0 < \delta < \eta$ with $1/(\eta - \delta) = (1/\eta) + \epsilon'$. By (Definition 3.4, p. 121, [84]) we have $\underline{\lim}_{q\to\infty} q^{\eta-(\delta/2)}\langle q\beta - j\rangle = 0$ and thus

$$\langle q\beta\rangle < q^{-\eta+(\delta/2)}$$

for an infinite number of positive integers q. There are infinitely many positive integers q and p such that

$$|\beta - p/q| < q^{-1-\eta+(\delta/2)}.$$

That is, by choosing q large enough, we can always find a p such that $|q\beta - p| = \langle q\beta\rangle$. As q increases p/q is a better approximation to the irrational β. For θ some irrational with $|\theta| < 1$, we have

$$\beta = p/q + \theta q^{-1-\eta+(\delta/2)}.$$

Pick a q such that the above relations are valid. Set

$$N = \left[q^{j(\eta-\delta)}\right].$$

Then for $1 \leq n^j \leq N^{1/j}$,

$$n^j\beta = n^j(p/q) + \theta_n,$$

with

$$\begin{aligned}|\theta_n| &= \left|n^j\theta q^{-1-\eta+(\delta/2)}\right| \\ &< n^j q^{-1-\eta+(\delta/2)} \\ &\le q^{[j(\eta-\delta)]^{1/j}-1-\eta+(\delta/2)} \\ &= q^{-1-(\delta/2)}.\end{aligned}$$

Thus, none of the fractional parts $\{\beta\}$, $\{2^j\beta\}$, $\ldots$, $\{\left[N^{1/j}\right]\beta\}$ lie in the interval $J=\left[q^{-1-(\delta/2)}, q^{-1}-q^{-1-(\delta/2)}\right)$, so

$$D_N(\omega_j) \ge \left|\frac{A(J,N)}{N}-\lambda(J)\right| = \lambda(J),$$

where $\lambda(J)$ is simply the "size" of the set J. For large enough q, we have $\lambda(J) \ge 1/2q$. But from the definition of N it is clear that

$$N \le q^{j(\eta-\delta)} \le N+1 \le 2N,$$

so

$$q^{-1} \ge cN^{-[j(\eta-\delta)]^{-1}}.$$

Combining these inequalities, we obtain

$$\begin{aligned}D_N(\omega_j) &\ge c'N^{-[j(\eta-\delta)]^{-1}} \\ &= c'N^{-(1/j)(1/(\eta-\delta))} \\ &= c'N^{-(1/j)((1/\eta)+\epsilon')} \\ &= c'N^{-(1/\eta j)-\epsilon}\end{aligned}$$

where $\epsilon=\epsilon'/j$. That is, we have shown, for all $\epsilon>0$, that

$$D_N(\omega_j)=\Omega\left(N^{-(1/\eta j)-\epsilon}\right).$$

□

7.4.3 Combescure's conjecture, Bourget's work and new results

Before discussing the conjecture, we must clearly understand Combescure's proof for the harmonic oscillator case. As stated in Section 7.3, the aim is to show that

$$B^{-1}(x) = \sum_{n=0}^{\infty} |a_n|^2 \left(\frac{2}{\sin(x-\theta_n)} \right)^2 \to \infty.$$

Define the set $S(x)$,

$$S(x) = \{n : |x-\theta_n| \leq |a_n| = n^{-\gamma} 2\pi\}. \tag{7.11}$$

Each n is an element of $S(x)$ if x is "close to θ_n". Note that $\theta_n = 2\pi\{\alpha_n/2\pi\hbar\}$, where $\{.\}$ is the fractional part, not "set" and α_n are the eigenvalues of the base Hamiltonian H_0.

Given that $\sin x \leq x$ for all $x \geq 0$, Combescure obtains a lower bound for $B^{-1}(x)$,

$$\begin{aligned} B^{-1}(x) &\geq \sum_{n=0}^{\infty} |a_n|^2 \left(\frac{2}{x-\theta_n} \right)^2 \\ &\geq \sum_{n\in S(x)} \frac{4|a_n|^2}{(x-\theta_n)^2} \geq 4\#S(x). \end{aligned} \tag{7.12}$$

Each $n \in S(x)$ gives a contribution to the sum of greater than one as $|a_n|/|x-\theta_n| \geq 1$. By only considering $\#S(x)$, we simply count a "1" each time.

The results on the discrepancy of sequences are now used, with the sequence $\omega_{\text{HO}} = (\theta_n/2\pi)$. Note that each element of the sequence ω_{HO} is in $[0,1)$.

Consider the interval, defined for every $x \in (0, 2\pi)$ and centred around $x/2\pi$,

$$J_N(x) = \left[\frac{x}{2\pi} - N^{-\gamma}, \frac{x}{2\pi} + N^{-\gamma} \right]. \tag{7.13}$$

For large enough N, $J_N(x) \subset [0,1)$. The size of the interval is $2N^{-\gamma}$. Using this particular subset and noting that the definition of discrepancy (7.7) involves taking the supremum over all subsets of $[0,1)$, Combescure obtains

$$\left|N^{-1}A(J_N(x),N)-2N^{-\gamma}\right|\leq D_N(\omega_{\text{HO}}).$$

Multiplying through by N gives

$$\left|A(J_N(x),N)-2N^{1-\gamma}\right|\leq ND_N(\omega_{\text{HO}}). \tag{7.14}$$

As $|\psi\rangle\notin l_1(H_0)$

$$\sum|a_n|\to\infty$$

and thus

$$1/2<\gamma\leq 1$$

from simple convergence arguments. Therefore, $N^{1-\gamma}$ grows at a rate[4] less than $N^{1/2}$. At this stage, Combescure utilises the theorems discussed above on the discrepancy of sequences. For the eigenvalue sequence, $\alpha_n=n\hbar\omega$, of the harmonic oscillator[5] the $j=1$ case of Theorem 7.9 applies which is exactly (Theorem 3.2, [84]). Combescure obtains the result[6]

$$D_N(\omega_{\text{HO}})=O(N^{-1/\eta+\epsilon}).$$

For the sequence ω_{HO}, $\beta=\omega/2\pi$. If β is an irrational of constant type ($\eta=1$), the strongest type of irrational, then

$$ND_N(\omega_{\text{HO}})=O(N^{\epsilon}).$$

[4]Interestingly, it can in fact not grow at all ($\gamma=1$) which is a subtle point seemingly missed by Combescure and others. The rank-1 projection operator from the vector $|\psi\rangle$ constructed with $\gamma=1$ is not shown to lead to the emergence of a continuous spectrum. Therefore, the statement that $|\psi\rangle\notin l_1(H_0)$ implies $|\psi\rangle\in\mathcal{H}_{\text{cont}}$ is not in fact proved to be true. There are states not in $l_1(H_0)$ that may not be in the continuous spectrum. In practice (numerical, experimental work) this should not cause any trouble. It is clearly easy to avoid $\gamma=1$.

[5]Do not confuse ω, the harmonic oscillator frequency, with ω_{HO}, the label for the sequence in $[0,1)$, the discrepancy of which is being bounded.

[6]This is not based on a conjecture as for $j=1$ a direct proof is possible, bypassing Conjecture 7.7. See [84].

As the right-hand side of (7.14) can be made to grow arbitrarily slowly, we conclude that the left-hand side must grow slowly too. Thus, to cancel the growth of $2N^{1-\gamma}$, $A(J_N(x), N)$ must grow at a rate arbitrarily close to that of $2N^{1-\gamma}$. We see that

$$A(J_N(x), N) \to \infty$$

as $N \to \infty$. It is now a simple observation [28] that this implies that $\#S(x) \to \infty$ and thus $B^{-1}(x) \to \infty$. Thus, e^{ix} is in the continuous spectral subspace of the Floquet operator V.

The importance of the eigenvalue sequence is seen in that if we cannot limit the right-hand side of (7.14), then we cannot place a lower limit on $A(J_N(x), N)$ and thus we cannot conclude that $B^{-1}(x) \to \infty$. Two barriers to limiting the right-hand side of this equation exist—j and η. If, still in the harmonic oscillator case, we wished for $\beta = \omega/2\pi$ to only be of a weaker type, say $\eta = 2$, we would no longer be able to conclude that $B^{-1} \to \infty$. The right-hand side would grow like $N^{1/2+\epsilon}$, which is always faster than $2N^{1-\gamma}$ for $1/2 < \gamma \leq 1$ which grows at a rate of $N^{1/2-\epsilon}$. Thus, no suitable lower limit for $A(J_N(x), N)$ can be found. Similarly, if the eigenvalue sequence is generalised (Combescure's conjecture) then we run into trouble. For $j = 2$, the lowest possible growth rate for the right-hand side we can obtain, taking Conjecture 7.7 as true, applying Theorem 7.9 and noting Theorem 7.10 which says we cannot do any better, is, once again, $N^{1/2+\epsilon}$. For larger j, the situation only gets worse.

Given these seemingly significant problems, the natural question to ask is: "How does one get around this problem?". The answer is provided in the work of Bourget [15]. Bourget proves a weaker theorem than Combescure's conjecture. Where Combescure kept the same requirement on $|\psi\rangle$, that it be in $l_1(H_0)$, Bourget has a j-dependent requirement. Essentially, for increasing j the a_n terms used to construct $|\psi\rangle$ must decrease more slowly with n. See Bourget's work [15] for the exact requirement, which depends on the best estimates available for Weyl sums discussed earlier and thus is a non-trivial function of j.

The key insight in obtaining the proof is to modify the set $S(x)$ (equation (7.11)) and the corresponding interval $J_N(x)$ (equation (7.13)) that are considered. Importantly, they become j-dependent. Bourget reduces the shrinking rate of the set $J_N(x)$ as a function of N just enough so as to allow the weaker limits on the discrepancy to be good enough to force the right-hand side of the equivalent to (7.14) to be less than the left-hand side, while keeping strong enough control on terms in the new set $S(x)$ to still argue that $B^{-1} \to \infty$.

Using the best available estimations on Weyl sums and plugging these into the upper bound formulas for discrepancy (as discussed earlier when introducing the work by Vinogradov), Bourget manages to provide a rigorous proof of the existence of a continuous spectral component of the Floquet operator (the essence of Combescure's conjecture) for $j \geq 3$, leaving only the $j = 2$ case unresolved. The proof is, unfortunately, unavoidably clouded by the "messy" estimates available for Weyl sums and thus, the essence of the proof is difficult to see. Here, I will revisit the proof, but (utilising Conjecture 7.7) apply Theorem 7.9 which says (using 2ϵ, rather than ϵ for technical reasons), for all $\epsilon > 0$

$$D_N(\omega) = O\left(N^{-(1/\eta j)+2\epsilon}\right).$$

With this very clean estimate, it is far easier to see how Bourget's work provides a proof that a continuous spectral component of the Floquet operator exists. It also extends the result to $j = 2$. Of course, the $j = 2$ case remains unproved as I have relied upon Conjecture 7.7, but I highlight the fact that a solution to Vinogradov's conjecture would solve Combescure's physics conjecture. I have also simplified the j-dependence of the a_ns used to construct $|\psi\rangle$.

THEOREM 7.11 *Assume Conjecture 7.7 is true and thus Theorem 7.9 follows.*

Assume β is irrational and of type η. Then for all positive integers, j, the Floquet operator, V, has $\sigma_{cont}(V) \neq \emptyset$ if $1/2 < \gamma < 1/2 + 1/2\eta j$.

Proof. (7.11) The proof relies upon the techniques utilised by Bourget. In essence, we simply increases the size of the interval (equation (7.13)) from $2N^{-\gamma}$ to $2N^{2(1/2-\gamma)}(\log N)^{-1/2}$. The important change is the first factor. The $\log N$ term is essential for technical reasons, but has a negligibly small effect on the shrinkage rate of the interval for large N. As $\log N/N^{4\delta} \to 0$ as $N \to \infty$ for all $\delta > 0$, for N large enough we have

$$2N^{2(1/2-\gamma)}(\log N)^{-1/2} > 2N^{2(1/2-\gamma-\delta)}.$$

Using this underestimate for the size of the interval, we easily obtain the equivalent of (7.14),

$$\left|A(J_N(x), N) - 2N^{2(1-\gamma-\delta)}\right| \leq ND_N(\omega_j),$$

for the sequence $\omega_j = (n^j\beta)$. Now, using Theorem 7.9, it is evident that to ensure $A(J_N(x), N) \to \infty$, we must have

$$2(1-\gamma-\delta) > 1 - (1/\eta j) + 2\epsilon,$$

or

$$\gamma < 1/2 + (1/2\eta j) - \epsilon - \delta.$$

The condition

$$1/2 < \gamma < 1/2 + (1/2\eta j), \tag{7.15}$$

where the "$<$" sign has absorbed the arbitrarily small numbers ϵ and δ, must be satisfied to force $A(J_N(x), N) \to \infty$.

Finally, we must show that $B^{-1}(x) \to \infty$ when this larger interval is used. Corresponding to the new interval $J_N(x)$, we introduce the new set $S(x)$,

$$S(x) = \left\{n : |x - \theta_n| \leq 2\pi N^{2(1/2-\gamma)} \log N^{-1/2}\right\}.$$

The estimate (7.12) is the same, except with the new set $S(x)$, which no longer has all terms greater than unity. Thus, it is not enough to simply count the number of terms in $S(x)$. A more subtle estimate is required. Replacing the numerator, $|a_n|$, with something smaller, $N^{-\gamma}$, and the denominator, $(x - \theta_n)$, with something larger, $2\pi N^{2(1/2-\gamma)} \log N^{-1/2}$, we obtain

$$B^{-1}(x) \geq \frac{1}{\pi^2} \sum_{n \in S(x)} \frac{\log N}{N^{2(1-\gamma)}},$$

which is essentially the estimate Bourget obtains. The estimate contained therein (Lemma 3.5 in [15]) then shows that $B^{-1}(x) \to \infty$ and the argument is complete. □

Examining (7.15) note that for $j = 1$ (for $\eta = 1$) we recover the simple result of Combescure. For all $j \geq 2$, we have a stronger (j-dependent) condition on $|\psi\rangle$ than simply $|\psi\rangle \notin l_1(H_0)$. This complication is the main weakening of Combescure's conjecture that Bourget and I have been forced to make. Note that the restriction on γ takes into account the end point subtleties referred to in the preceding discussions.

I have replaced the requirement that $|\psi\rangle \notin l_1(H_0)$ (i.e., $1/2 < \gamma \leq 1$) with the j-dependent requirement $1/2 < \gamma < 1/2 + (1/2j)$. In Bourget's work, the requirement is stronger—directly related to the replacement of the known limits on Weyl sums (in terms of ρ in the earlier sections) with the "best possible" estimate from our Conjecture 7.7 of $(1/j) - \epsilon$.

7.4.4 Summary

Reliance on Conjecture 7.7 and the result of Theorem 7.9 derived from it has allowed me to discuss Bourget's proof without the complications of the messy estimations on Weyl sums. This simplified discussion highlights the key aspects of Bourget's proof. It has also shown that the $j = 2$ case for the emergence of a continuous spectral component of the Floquet operator is solved by Vinogradov's conjecture. A proof of Vinogradov's conjecture is no longer just of mathematical interest. It has a direct mathematical physics consequence.

Finally, note that the rank-N equivalent of this work follows in the same way as presented for the harmonic oscillator case in Section 7.3, providing a complete rank-N generalisation of the work of Combescure [28].

7.5 Generalising the results of Milek and Seba

Having established that the continuous subspace of $\mathcal{H}$, $\mathcal{H}_{\text{cont}}$, is not empty, I now wish to characterise it—by identifying the singular and absolutely continuous components. Here, I extend the result of Milek and Seba to rank-N perturbations. I do not extend the numerical results of Milek and Seba as they rely on the assumption that the $j = 2$ eigenvalue spectra lead to a continuous Floquet spectrum—a result I have just shown to be as yet unjustified.

THEOREM 7.12 *Assume $H(t)$ is given by (7.1) and that (7.2) applies. Assume $B_k^{-1}(x) \to \infty$ and thus $\mathcal{H}_{cont} \neq \emptyset$. Then $\mathcal{H}_{ac} = \emptyset$ and thus $\mathcal{H}_{sc}$ is not-empty. The Floquet operator, V, has a non-empty singular continuous spectrum.*

Proof. (7.12) As shown in the proof of Theorem 6.4a and easily calculated, the Floquet operator can be written in the form

$$V = U + \sum_{k=1}^{N} R_k,$$

where

$$R_k = \left(e^{i\lambda_k/\hbar} - 1\right) |\psi_k\rangle\langle\psi_k| U. \tag{7.16}$$

We can now use either (Theorem 5, Howland [65]) or (Theorem 1, Birman and Krein [8]). The theorem from the paper of Birman and Krein is more direct, so we use it here. It states that if we have two unitary operators, U and V, that differ by a trace class operator, then the wave operators

$$\Omega_{\pm} = \text{s-}\lim_{\nu\to\pm\infty} V^{\nu}U^{-\nu}P_{\text{ac}}(U)$$

exist and their range is the absolutely continuous subspace of V,

$$R(\Omega_{\pm}) = \mathcal{H}_{\text{ac}}(V). \tag{7.17}$$

We must show that the difference $V - U$ is finite. With the notation in Chapter 6, where the perturbation W is given by A^*A and

$$A = |\psi\rangle\langle\psi|,$$

with

$$|\psi\rangle = \sum_n a_n\phi_n,$$

we obtain

$$\begin{aligned}
\operatorname{Tr} A^*A = \operatorname{Tr} A &= \sum_l \langle\phi_l|A|\phi_l\rangle \\
&= \sum_{l,m,n} \langle\phi_l|a_n|\phi_n\rangle\langle\phi_m|a_m^*|\phi_l\rangle \\
&= \sum_{l,m,n} a_n a_m^* \delta_{ln}\delta_{ml} \\
&= \sum_l |a_l|^2 = 1
\end{aligned}$$

as $|\psi\rangle \in l_2(H_0)$ and is normalised. The perturbation to the Hamiltonian is trace class. The difference in unitary operators, U and V, is also trace class. By the triangle inequality for norms,

$$\|R_k\|_{\text{tr}} \leq \|\left(e^{i\lambda_k/\hbar} - 1\right)\| \| |\psi_k\rangle\langle\psi_k| \|_{\text{tr}} \|U\|_{\text{tr}} \ .$$

As $\|U\|_{\text{tr}} = 1$,

$$\begin{aligned}\operatorname{Tr}\left(\sum_{k=1}^{N} R_k\right) &\leq \sum_k \|(e^{i\lambda_k/\hbar} - 1\| \sum_{l,m,n} \langle\phi_l|(a_k)_n|\phi_n\rangle\langle\phi_m|(a_k)^*_m|\phi_l\rangle \\ &= \sum_k \left|e^{i\lambda_k\hbar} - 1\right| \\ &= \sum_k \sqrt{2(1 - \cos\lambda_k/\hbar)}.\end{aligned}$$

Armed with a trace-class perturbation, we conclude that the wave operators exist. The existence of the operators $\Omega_\pm$ means that they are defined for all states in the Hilbert Space $\mathcal{H}$. Note (equation (7.17)) that the subspace $\mathcal{H}_{\text{ac}}(V)$ is equal to the range of these operators. However, $P_{\text{ac}}(U)$ gives zero when acting on any state in $\mathcal{H}$ because U is pure point. Thus, $\mathcal{H}_{\text{ac}}(V)$ is empty. As $\mathcal{H}_{\text{cont}}$ is not empty, $\mathcal{H}_{\text{sc}}$ must be non-empty, and we have proved that a singular continuous subspace of the Floquet operator V exists. □

The key assumption in Theorem 7.12 is that $B_k^{-1}(x) \to \infty$. This is certainly true for $j = 1$ if $|\psi_k\rangle \neq l_1(H_0)$. For $j \geq 2$ the results were discussed in detail in Section 7.4. For $j \geq 3$, Bourget showed that one can construct vectors $|\psi_k\rangle$ for which $B_k^{-1}(x) \to \infty$. I have shown, in Conjecture 7.11, that if Conjecture 7.7 is true then this result extends to $j \geq 2$ and with improved requirements on the states $|\psi_k\rangle$.

7.5.1 Discussion

Milek and Seba make a number of incorrect statements in obtaining this result for the rank-1 case. Firstly, they state that the operator[7] $R = [\exp(i\lambda/\hbar) - 1]\,|\psi\rangle\langle\psi|U$ is rank-1 which it is not—the presence of the unitary operator U stops R from being rank-1. This is not, however, important. The applicability of the theorems

[7] As we are dealing with the rank-1 case, the subscript k may be dropped from (7.16).

in [65, 8] does not rely upon the rank of the operator R, but upon it being of trace-class. Secondly, they claim that the existence of the wave operators implies that

$$\sigma_{\text{ac}} V \subset \sigma_{\text{ac}}(U). \tag{7.18}$$

This is, again, not true. Given that $\sigma_{\text{ac}}(U)$ is empty, it is indeed possible to conclude that $\sigma_{\text{ac}}(V)$ is empty, as discussed above, but the relation (7.18) does not follow. Consider the situation where $\sigma_{\text{cont}}(U)$ is not empty. Then there is a set of vectors in $\mathcal{H}$ which are continuous for U. These vectors form the domain for the operator V^ν in the wave operators. The action with V^ν does not however keep us in the subspace $\mathcal{H}_{\text{cont}}(U)$ as the space we get to (the range for V^ν) is only invariant for $\mathcal{H}_{\text{cont}}(V)$, not $\mathcal{H}_{\text{cont}}(U)$. Thus, we may obtain a vector, necessarily in $\mathcal{H}_{\text{cont}}(V)$ due to invariance, but possibly in $\mathcal{H}_{\text{s}}(U)$, and thus, we cannot conclude that $\sigma_{\text{ac}}(V) \subset \sigma_{\text{ac}}(U)$. These two points discussed do not make the final results of Milek and Seba wrong, but "only" the proofs.

Of greatest concern is the use of (Lemma 6, Combescure [28]) without justification. Milek and Seba have assumed that Combescure's conjecture is true. Bourget's demonstration that a continuous spectral component of the Floquet operator exists does not cover the $j = 2$ case which is exactly the situation in Milek and Seba's paper. Furthermore, I have shown that, using the "best possible" cases for discrepancy, the $j = 2$ case is covered, but, as I relied on Conjecture 7.7, I have not actually proved it. It is worrying that Milek and Seba's work remains unjustified.

7.6 Summary

I have generalised the work of both Combescure [28] and Milek and Seba [90] from rank-1 to rank-N. I have also discussed in detail Combescure's conjecture, my work on estimations of discrepancy and the demonstration by Bourget [15] that a continuous spectral component of the Floquet operator does exist for certain constructions of $|\psi\rangle$. This covers the essential aim of Combescure's conjecture on the existence of a continuous spectral component. A clear view of the essence of Bourget's proof has been provided by taking a reasonable number-theoretic conjecture to be true. With this clear view, the work of Bourget becomes more accessible. I also demonstrated that reliance on Vinogradov's conjecture allows one to extend the work to the $j = 2$ case, showing that a proof of Vinogradov's conjecture would have direct implications in mathematical physics.

An in depth critical analysis of the work of Milek and Seba was also undertaken; I highlighted a number of misconceptions and errors in the work. I have also highlighted that, even with Bourget's demonstration of the existence of a continuous spectral component of the Floquet operator for $j \geq 3$, Milek and Seba's work *still* is not fully justified. Using Vinogradov's conjecture, one can then justify Milek and Seba's result. A direct proof of Combescure's conjecture or a proof of Vinogradov's conjecture, allowing my work to bridge the gap, remains desirable.

Chapter 8

Conclusions and Further Work

Contents

In this thesis I have presented new results on the classification of the spectrum of the Floquet operator for a class of kicked Hamiltonian systems.

Before presenting the main results, I reviewed the fields of classical and quantum chaos (Chapter 2) and presented a detailed investigation of the links between quantum dynamics and spectral analysis (Chapter 5). A point of ambiguity in the physics literature was also identified and commented on.

In Chapter 4 I provided a conceptual introduction to the mathematical field of spectral and functional analysis, highlighting the physical meaning behind much of the basic mathematical building blocks. The aim was not only to lay the groundwork for the material in Chapter 6, but to make this important field of mathematics more accessible to physicists. An appreciation of functional and spectral analysis provides one with a deeper understanding of basic quantum mechanics.

In Chapter 6 I developed a number of unitary equivalent theorems to those well known in the self-adjoint theory (e.g., the Putnam–Kato theorem) and successfully applied them to show that the spectrum of the Floquet operator remains pure point (given that $U = e^{-iH_0T}$ has pure point spectrum) when the perturbation is suitably constrained. It should be stressed that the result is non-perturbative. I also obtained this result in a more straight forward, but less general, way by extending the work of Combescure. This was presented in the early parts of Chapter 7.

In the remaining sections of Chapter 7 I extended the results on the emergence of a continuous spectrum of the Floquet operator to rank-N perturbations and investigated Combescure's conjecture that the eigenvalue sequence for the unperturbed Hamiltonian, H_0, should not affect the results in a significant way. Reviewing the work of Bourget and linking it to a number-theoretic conjecture put forward by Vinogradov, I showed that if one could solve Vinogradov's conjecture, then the essence of Combescure's conjecture would follow. For any eigenvalue sequence for H_0 described by a polynomial, a continuous component will emerge under realisable conditions for the rank-N operator perturbation.

8.1 Future directions

The clearest loose end in the work presented in this thesis would be to find a proof of Vinogradov's conjecture on the estimation of Weyl sums. Without a proof, it seems reasonable to conclude that the work of Milek and Seba on kicked rotors and the existence of a continuous component cannot be properly justified. Having stood for over fifty years, a proof or disproof seems unlikely to turn up any time soon.

When considering open questions of physical, rather than mathematical, interest, a different direction is seen for extending this work. It is broadly acknowledged that moving beyond the closed system dynamics governed by the Schrödinger equation is of great use in analysing chaos in quantum systems and investigating the quantum–classical correspondence. Thus, it would be interesting to allow for environmental interactions and to study the behaviour of kicked systems in so called "open quantum systems". There is already a great deal of research effort in open systems and specifically, the analysis of kicked systems in such environments. Many of the results look promising. Applying the techniques developed in this work would be interesting.

Returning to the closed system dynamics, an extension of the work presented in Chapter 6 to infinite N would be valuable. Similar work for the Hamiltonian system was done in the later part of Howland's paper [66]. As $N \to \infty$ a number of the tools and arguments used for finite N clearly collapse and one must be rather cautious. The physical implications of infinite N systems are also open to investigation.

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