# Applications of Functional Analysis in Quantum Scattering Theory


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I declare that this thesis is my own account of my research and contains as its main content work which has not been previously been submitted for a degree at any university.

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# Abstract

The aim of this thesis is to present a reasonable account of some of the applications that functional analysis, or more specifically operator theory, has in the theory of quantum scattering. We begin by introducing the physical scattering experiment as well as establishing the standard framework for discussing quantum theory, that of a Hilbert space. This leads to a discussion of the properties of operators acting in a Hilbert space and the role played by unbounded self-adjoint operators in quantum physics. We also spend some time discussing the position, momentum and energy operators which are of most relevance here. This in turn leads logically to the problem of formulating the scattering problem mathematically using these operators. The *stationary* equations of scattering theory are also rigorously derived and their suitability for two-body scattering problems is proven. We show that this analysis does not extend to three-body scattering problems, and introduce the *Faddeev* formulation for three-body systems to supplement the theory. This thesis concludes with a brief overview of how our scattering equations can be modified to take into account effects such as particle spin and identical particles, before discussing an example of a three-body scattering problem (incorporating these features) and deriving a mathematically satisfactory set of equations which are amenable to numerical solution.

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I should also take this opportunity for a couple of apologies. I apologise to all physicists for not using the Dirac notation. I also apologise to all mathematicians for stubbornly insisting on writing inner-products the wrong way around. I guess if you can’t please everyone, you might as well please nobody...

# Contents

# Chapter 1

# Introduction

*"The beginner should not be discouraged if he finds that he does not have the prerequisites for reading the prerequisites."*
P R Halmos

## 1.1 Quantum Scattering - an Outline

### 1.1.1 Quantum Theory

Quantum theory was developed early in the twentieth century in an attempt to explain physical phenomena which could not be explained using the familiar classical theory. Examples include black-body radiation, the photo-electric effect and why electrons did not spiral into the nucleus. Contributors to the early theory include such famous names as Planck, Einstein, Bohr, Sommerfield and de Broglie. However, it was Heisenberg who first proposed what was to become quantum theory and his formulation was based on the principle that in any physical theory, one should distinguish between quantities that are observable and those which are not. Since we can only test theories by observation, he demanded that a satisfactory theory should be founded on observables, and that non-observables in the theory may be modified or removed without affecting any theoretical predictions.

Heisenberg then proceeded to construct such a theory of the atom. A partially successful model at the time due to Bohr relied upon the concept of the orbit of an electron around the nucleus. Heisenberg argued that this was unsatisfactory since it was known that the radius of the orbit could not be accurately measured. Instead, he developed a theory based on the frequencies of radiation emitted by atoms. These are accurately observable. The theory became known as *matrix mechanics* after mathematicians realised that his theory relied upon the multiplication of matrices [47].

At about the same time, Schrödinger formulated his *wave mechanics*. This was based upon the ideas of de Broglie - namely that matter could have a wave-like nature just as waves were being shown to have particulate natures. Schrödinger postulated that matter waves could be represented by a *wavefunction* $\Psi(t)$ which obeyed the dynamical law of motion

$$i\bar{h}\frac{\partial\Psi}{\partial t} = H\Psi \tag{1.1}$$

where $\bar{h}$ is Planck's constant divided by $2\pi$ and $H$ is an operator called the *Hamiltonian* representing the energy of the system. This is, of course, the much celebrated *Schrödinger Equation*. We shall return to this equation later. For now, we shall mention that in simple cases, $H$ can be decomposed into the sum of a *kinetic energy operator* $H_0$ and a *potential energy operator* $V$ which are such that $H_0 = p^2/2m$ and $V = V(x)$ where $p$ is the *momentum operator*, $m$ is the mass of the system (not an operator) and $V(x)$ is a function of the *position operator* $x$.

### 1.1.2 The Scattering Concept

Scattering experiments are most important in quantum physics, not only as a means of providing experimental data to test theories upon but also as a means of producing the particles of interest themselves. Indeed, the development of quantum theory was in a sense, catalysed by scattering experiments. For instance, the existence of the nucleus was proven by Rutherford using $\alpha$-particle scattering off gold atoms, and the existence of discrete atomic energy levels was shown by Franck and Hertz using the scattering of electrons off mercury atoms [45]. Even the familiar chemical reactions taking place in industry and laboratories all over the world are just glorified (that is, extremely complicated) scattering experiments.

The simplest example of scattering is where an elementary particle "collides with" or is scattered by a fixed target. The experimental quantity of interest will be the probability that the particle will be scattered into a particular region of space (ie into a particular range of solid angles). This can be measured in the laboratory by taking a large number of these collisions (for instance by using a collimated beam of the incident particles) and measuring the intensity of the resulting particles at different points in space. A structural diagram is shown below in figure 1.1.

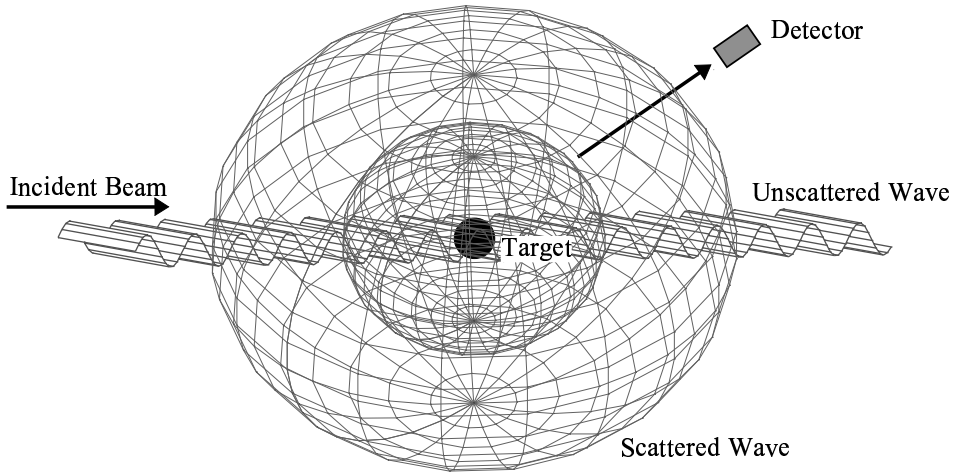


Figure 1.1: A *stationary* or time independent view of a scattering experiment.

From a theoretical point of view, the aim is to be able to calculate what these probabilities will be. The simple approach is to start with the incident wavefunction (we are implicitly working in Schrödinger's representation), write down the Hamiltonian of the system $H$, substitute into the Schrödinger equation and then solve to find the final wavefunction. Sounds easy, doesn't it?

Unfortunately, it isn't. The Schrödinger equation is extremely difficult to solve in general as the appropriate boundary conditions are not easy to formulate. Even the satisfactory mathematical formulation of an arbitrary scattering problem must rank as one of the hardest problems in mathematical physics, and indeed, it has not yet been solved in generality. Recent progress is documented in [23]. It is also well known that the Schrödinger equation can be transformed into other equations which give the pertinent information, but these equations too generally aver solutions.

The theory needed to adequately describe the scattering phenomenon is of mathematical interest, not only for its difficulty but because it encompasses such a variety of mathematical disciplines ranging from the pure to the very applied and even probabilistic. In the course of this thesis, some of the mathematical theory appropriate for this description will be described. This will then be applied to the simplest scenario, that of one or two particle scattering, to derive mathematically the equations of scattering theory and to examine the conditions necessary for a

rigorous formulation. The remainder of the thesis will deal with the more complicated problem of three-body scattering and the far greater difficulties that this problem poses mathematically. We then discuss the method by which satisfactory three-body scattering equations were first derived (the *Faddeev* formulation) before examining a specific (simple) three-body scattering problem using this approach.

## 1.2 Some Mathematical Preliminaries

### 1.2.1 Hilbert Space

Let us begin by defining an inner-product which we shall denote by $\langle \cdot, \cdot \rangle$. We require an inner-product over a vector space $V$ to be a complex-valued function with the following properties for any $f, g, h \in V$ and any scalar $\alpha$:

$$\begin{aligned} \langle f, f \rangle &\geqslant 0 \quad \text{and} \quad \langle f, f \rangle = 0 \quad \text{iff} \quad f = 0, \\ \langle f, g+h \rangle &= \langle f, g \rangle + \langle f, h \rangle, \\ \langle f, \alpha g \rangle &= \alpha \langle f, g \rangle, \\ \langle f, g \rangle &= \overline{\langle g, f \rangle}. \end{aligned}$$

We note that we use the convention common in physics that the inner-product is linear in the second argument and conjugate-linear in the first. This is the opposite of the convention used in mathematics.

A vector space equipped with an inner-product space is naturally called an *inner-product space* (also termed a *Euclidean space* or a *pre-Hilbert space*). Any inner-product space has a norm $\| \cdot \|$ defined by

$$\| f \| = \sqrt{\langle f, f \rangle}.$$

The distance between two vectors $f$ and $g$ (*in norm*) is given by $\| f - g \|$. If the inner-product space also has the property that any sequence whose terms get arbitrarily close in norm do actually converge to some vector (the *completeness* property) then it is called a *Hilbert space*. We shall often denote an arbitrary Hilbert space by $\mathscr{H}$.

It is well established that the mathematical formulation of quantum theory uses an abstract Hilbert space to represent the system in question, the vectors, usually termed *state vectors*, then represent the set of allowed wavefunctions (zero is excluded for probabilistic reasons). It is also common in elementary textbooks to demand that state vectors must have norm 1. Although this has the advantage of simplifying some calculations, it is not necessary and we shall not impose this demand in this thesis.

Why we use a Hilbert space is not physically clear and some efforts have been made to clarify this issue. Most are based on the idea of a *lattice of propositions* wherein the elements of the lattice are yes/no answerable experiments and the partial ordering is implication (ie a yes answer for this experiment implies a yes answer for another). This is hoped to produce a Hilbert space structure and an introductory treatment is given in [24]. Another demand generally made is that the underlying Hilbert space should be separable. However, this demand seems to be employed because no urgent need for non-separable Hilbert spaces has yet surfaced in non-relativistic quantum theory.

A *separable* Hilbert space, $\mathscr{H}$, is one which has a countable subset $S$ that is dense in $\mathscr{H}$ (that is, the closure of $S$ is $\mathscr{H}$ itself). The importance of this concept is that a separable Hilbert space possesses a countable *orthonormal basis* (also known as a total orthonormal set) $\{e_1, e_2, \ldots\}$ which have the properties that $\forall f \in \mathscr{H}$,

$$\langle e_k, f \rangle = 0 \quad \forall k \quad \Rightarrow \quad f = 0 \qquad ; \qquad f = \sum_{k=1}^{\infty} \langle e_k, f \rangle \, e_k. \tag{1.2}$$

That is, the only vector orthogonal to the orthonormal basis is the zero vector and any vector can be expanded in a countably infinite sum with respect to the orthonormal basis.

### 1.2.2 Measure Theory

The theory of measures can be thought of for our purposes as a theory of integration. A measure $\mu$ is a real-valued function defined on a class $M$ of subsets (actually a $\sigma$-algebra called the $\mu$-*measurable* sets) of any set $S$, which is non-negative, countably sub-additive and is zero on the empty set $\varnothing$. A measure $\mu$ on $S$ gives rise to the notion of the integral of a function, $f$, over any measurable subset $A \in M$ which we shall denote by $\int_A f d\mu$ or by $\int_A f(x)\, d\mu(x)$. In this thesis, $S = \mathbb{R}^n$. For now, we shall be content to mention two examples of a measure. The *Lebesgue measure* generalises the familiar Riemann concept of integration in that the Lebesgue integral is defined on a larger class of functions and is equal to the Riemann integral when the latter is defined. We shall usually denote integration with respect to the Lebesgue measure by $dx$. The *counting measure* is defined on $\mathbb{R}$ by

$$\mu_C(A) = \left|A \cap \mathbb{Z}^+\right|.$$

That is, the number of positive integers in the set $A$. It is not hard to show that

$$\int_{\mathbb{R}} f(x)\, d\mu_C(x) = \sum_{k=1}^{\infty} f(k)$$

so that summations and integrations can be treated using the same general theory. The proofs of these statements and further theory are to be found in [19] or [34].

We can now adequately describe two of the most important Hilbert spaces in quantum theory. We denote by $L^2(\mathbb{R}^n, \mu)$ the vector space of all *complex-valued* ($\mu$-measurable) functions $f$ such that $\int_{\mathbb{R}^n} |f|^2 d\mu < \infty$, equipped with the inner-product:

$$\langle f, g \rangle = \int_{\mathbb{R}^n} \overline{f} g d\mu.$$

It turns out that with a measure $\mu$, such an inner-product space is complete. This would not be the case if we were to use the Riemann integral. If in addition, $\mu$ is $\sigma$-*finite* ($\mathbb{R}^n$ can be covered by a countable number of sets of finite measure) then $L^2(\mathbb{R}^n, \mu)$ is separable [38].

Of particular interest in quantum theory are the corresponding $L^2$ spaces with the Lebesgue measure, denoted by $L^2(\mathbb{R}^n)$, and with the counting measure, denoted by $\ell^2$, (the set of all square-summable complex-valued sequences). Both are clearly $\sigma$-finite, so both are separable Hilbert spaces. The importance of these spaces in quantum theory derives from the fact that Heisenberg's matrix mechanics was seen to be abstract quantum theory realised in the Hilbert space $\ell^2$, and Schrödinger's wave mechanics was seen to be abstract quantum theory realised in $L^2(\mathbb{R}^n)$ [31]. It is not hard to show that these two spaces are isomorphic, as are all infinite dimensional separable Hilbert spaces. Since all the physical information is given by inner-products in both formulations (see section 1.2.6), the two formulations are equivalent.

Other technically useful results in mathematical physics include the solution of the problems of when limits and integrals can be interchanged and when the order of integration of a multiple integral can be reversed. The solutions to these problems involving integration are naturally found using measure theory. Proofs of the following theorems may be found in any text on the subject (eg [19], [34]). We note first that a function $f$ is said to be *integrable* with respect to a measure $\mu$ if $\|f\|_1 = \int |f| d\mu < \infty$. The set of integrable functions over $\mathbb{R}^n$ is denoted by $L^1(\mathbb{R}^n)$. $L^1(\mathbb{R}^n)$ is not a Hilbert space but is complete with the norm $\|\cdot\|_1$. Also, if a condition is said to hold *almost everywhere* (ae) we mean that it holds everywhere with the exception of a set of measure zero. A set of measure zero contributes nothing to an integral so the phrase "almost everywhere" is ubiquitous whenever measure theory and integration are involved.

**Theorem 1 (Dominated Convergence)** *Suppose that $f_k$ converges pointwise ae and there exists $g \in L^1(\mathbb{R}^n)$ such that for all $k$, $|f_k(x)| \leq g(x)$ ae. Then,*

$$\lim_{k\to\infty} \int f_k d\mu = \int \lim_{k\to\infty} f_k d\mu.$$

**Theorem 2 (Fubini)** *Suppose that* $f \in L^1(\mathbb{R}^n)$. *Then,*

$$\int\int_{\mathbb{R}^n} f(x,y)\, d\mu_1(x)\, d\mu_2(y) = \int\int_{\mathbb{R}^n} f(x,y)\, d\mu_2(y)\, d\mu_1(x).$$

### 1.2.3 Operators on Hilbert Spaces

We shall define an *operator* on a Hilbert space $\mathscr{H}$ as a *linear transformation* from a linear subspace of $\mathscr{H}$ to $\mathscr{H}$. In quantum theory, it is generally assumed that any actual observable quantity of the system is mathematically represented by an operator of a specific kind. For instance, associated with the observable quantity "position", there is a corresponding position operator. A brief introduction to how these operators are related to the physically observed quantities is given in section 1.2.6.

We define a norm on the space of operators over a given Hilbert space. If $A$ is an operator then the norm of $A$ is given by

$$\|A\| = \sup_{f\neq 0} \frac{\|Af\|}{\|f\|} = \sup_{\|f\|=1} \|Af\|$$

where the norms under the suprema are the Hilbert space norms (the two definitions are easily shown to be equivalent). An operator with finite norm is a *bounded* operator and the set of all bounded operators over $\mathscr{H}$ is denoted by $B(\mathscr{H})$. From this definition, we immediately obtain $\|Af\| \leqslant \|A\|\,\|f\|$ for any $A \in B(\mathscr{H})$ and $f \in \mathscr{H}$.

As a specific example of how operators may be defined, let us consider the set of continuous linear functionals on $\mathscr{H}$. A functional $\phi(f)$ is a map from $\mathscr{H}$ to a scalar field, for us, $\mathbb{C}$, the set of complex numbers. The continuity requirement states that if $f_n \to f$ in $\mathscr{H}$, then $\phi(f_n) \to \phi(f)$ in $\mathbb{C}$. The set of continuous linear functionals on $\mathscr{H}$ is called the *dual* of $\mathscr{H}$, denoted $\mathscr{H}'$. We have the following important theorems proven in any text on functional analysis (eg [27][38], [42])

**Theorem 3 (Riesz)** *For every* $\phi \in \mathscr{H}'$, *there is a unique* $h \in \mathscr{H}$ *such that*

$$\phi(g) = \langle h, g\rangle \quad \forall g \in \mathscr{H}.$$

**Theorem 4 (Riesz Representation)** *If* $\phi \in (\mathscr{H}\times\mathscr{H})'$ *is sesquilinear, so that*

$$\begin{aligned} \phi(\alpha f + \beta g, h) &= \overline{\alpha}\phi(f,h) + \overline{\beta}\phi(g,h) \\ \textit{and}\quad \phi(f, \alpha g + \beta h) &= \alpha\phi(f,g) + \beta\phi(f,h) \end{aligned}$$

*for any* $f,g,h \in \mathscr{H}$ *and* $\alpha,\beta \in \mathbb{C}$ *then* $\phi$ *defines an operator* $A \in B(\mathscr{H})$ *by*

$$\langle f, Ag\rangle = \phi(f,g).$$

The second is derived from the first by noting that for fixed $g$, $\overline{\phi(f,g)}$ is a continuous linear functional in $f$ so there exists a unique $h \in \mathscr{H}$ such that

$$\overline{\phi(f,g)} = \langle h, f\rangle \quad \Rightarrow \quad \phi(f,g) = \langle f, h\rangle.$$

Of course, $h$ actually depends upon $g$. So we define an operator $A$ by $h = Ag$, hence the result.

### 1.2.4 Fourier Transforms and Distributions

The Fourier transform is an essential part of any study of quantum mechanics. A reference for many aspects of Fourier analysis relevant to mathematical physics is [40]. There are however, different definitions of the Fourier transform in common use. We shall follow the physical literature and take as our definition of the $n$-dimensional Fourier transform the following:

$$\widehat{f}(\mathbf{k}) = \int_{\mathbb{R}^n} f(\mathbf{r})\,\overline{\phi_{\mathbf{k}}(\mathbf{r})}\, d\mathbf{r} \tag{1.3}$$

and for the inverse Fourier transform:

$$f(\mathbf{r}) = \int_{\mathbb{R}^n} \widehat{f}(\mathbf{k})\, \phi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k} \tag{1.4}$$

where $\mathbf{r} = (x_1, \ldots, x_n)$, $\mathbf{k} = (k_1, \ldots, k_n)$ and $\phi_{\mathbf{k}}(\mathbf{r}) = (2\pi)^{-n/2} e^{i\mathbf{k}\cdot\mathbf{r}}$ is a function known to physicists as a *free plane wave*. We shall restrict $f$ to the space $S(\mathbb{R}^n)$, the set of rapidly decreasing functions. This are defined as the set of infinitely differentiable complex-valued functions over $\mathbb{R}^n$ for which $\sup|p(\mathbf{r})Df(\mathbf{r})| < \infty$ where $p(\mathbf{r})$ is any polynomial in $x_1, \ldots, x_n$ and $D$ is any differential operator of the form $\partial^a / (\partial x_1^{a_1} \ldots \partial x_n^{a_n})$. It should be noted that this is a subspace of the Hilbert space $L^2(\mathbb{R})$ but is by no means the largest such subspace for which the above definitions make sense. We shall also define the *Fourier operator* $F$ by $Ff = \widehat{f}$ for any $f \in S(\mathbb{R}^n)$. This definition will be extended in chapter 3.

We will also need to discuss the *Dirac delta function* $\delta(\mathbf{r})$. It is well known that this is not a function is the usual sense of the word but instead is described as a *distribution* (or *generalised function*). The class of distributions is defined as the dual space of a particular space of functions $T$, called test functions. Common choices for the test functions are the spaces $S(\mathbb{R}^n)$ [39] or $C_0^\infty(\mathbb{R}^n)$, the space of infinitely differentiable functions which are non-zero only on some bounded subset of $\mathbb{R}^n$ [14]. The (n-dimensional) Dirac delta function is defined as a functional by

$$\delta(\varphi) = \varphi(\mathbf{0}) \quad \forall \varphi \in T$$

which is often written in the form

$$\int_{\mathbb{R}^n} \delta(\mathbf{r})\, \varphi(\mathbf{r})\, d\mathbf{r} = \varphi(\mathbf{0}).$$

One of the important properties of the space of distributions is that the Fourier transform can be extended to distributions. In particular, it can be shown that in this distributional setting,

$$\widehat{\phi_{\mathbf{k}}}(\mathbf{k}') = \delta(\mathbf{k} - \mathbf{k}'), \tag{1.5}$$

so the Fourier transform of a free plane wave with momentum $\mathbf{k}$, is a Dirac delta function with a spike at $\mathbf{k}$. This corresponds to the intuitive idea that an ideal plane wave has an exact momentum (rather than a small range of momenta) so its transform will only be non-zero at one point.

### 1.2.5 A Touch of Topology

We should also like to briefly mention the subject of topology. Topology deals with the question of convergence in a very general sense. Without worrying about exactly what this means, we shall discuss briefly three topologies that can be defined on the operator space $B(\mathscr{H})$. What will be important to us is the question of convergence of operators in each of these topologies. This is of importance as results that may hold under one topology may be quite wrong in another. An excellent discussion of the properties of these topologies and some of the pitfalls encountered with naïve algebraic manipulations of operators is to be found in [20].

We shall define convergence in the *uniform topology* (also known as the *norm* or *operator* topology), the *strong topology* and the *weak topology*, respectively:

$$\begin{aligned}
A_k &\to A \text{ uniformly iff } \|A_k - A\| \to 0 \quad (A = \mathrm{u}\!-\!\lim_{k\to\infty} A_k) \\
A_k &\to A \text{ strongly iff } \|(A_k - A)f\| \to 0 \quad \forall f \in \mathscr{H} \quad (A = \mathrm{s}\!-\!\lim_{k\to\infty} A_k) \\
A_k &\to A \text{ weakly iff } |\langle g, (A_k - A)f\rangle| \to 0 \quad \forall f, g \in \mathscr{H} \quad (A = \mathrm{w}\!-\!\lim_{k\to\infty} A_k).
\end{aligned}$$

Technically, we should be defining convergence in terms of *nets* or generalised sequences. We shall not let this bother us however. It is immediately obvious that since $\|(A_k - A)f\| \leqslant$

$\|A_k - A\|\,\|f\|$, uniform convergence implies strong convergence. Also, using the Cauchy-Schwarz inequality, we have $|\langle g,(A_k-A)\,f\rangle| \leqslant \|g\|\,\|(A_k-A)\,f\|$ so strong convergence implies weak convergence.

In chapter 4 we will be working with the strong topology to derive certain results. However, it will be convenient to use the weak topology on occasion. We shall then appeal to the following simple lemma which will allow us to "return" to the strong topology [20].

**Lemma 5** *If $A_k \to A$ weakly and $\|A_k f\| \leqslant \|Af\|$ for all $f \in \mathscr{H}$ and $k > 0$, then $A_k \to A$ strongly.*

### 1.2.6 Linking Mathematics and Reality

It is generally accepted by most practising physicists that the abstract mathematics and the actual quantities measured in experiment and linked by what is called the *Born* (or *Copenhagen*) *interpretation*. In this interpretation, any physically observable quantity (say position of a system) is associated with an operator (call it $x$). If the system is in quantum state $\Psi$ at some time, experiments to determine the position of the system will in general yield different results but the mean result (called the *expected value*) is given by $\langle x\rangle = \|\Psi\|^{-2}\langle\Psi, x\Psi\rangle$ (the normalising factor of $\|\Psi\|^{-2}$ is usually absent in most quantum texts because it is implicitly assumed that all the quantum states are normalised such that $\|\Psi\| = 1$). We shall see shortly that for physical consistency, the operators that correspond to observable quantities must be of a particular class called the *self-adjoint* operators because these are guaranteed to give only real expectation values (remember that we work over a complex Hilbert space). The probability that a measurement lies within a set $B \subseteq \mathbb{R}$ is given by $\|\Psi\|^{-2}\langle\Psi, E^x(B)\,\Psi\rangle$ where $E^x(B)$ is an operator related to $x$ which depends on $B$, called the *spectral measure of* $x$. This operator belongs to the class of operators known as projectors which will also be discussed in more detail shortly. Projectors are also self-adjoint operators so we are again guaranteed real probabilities.

In essence, it is this idea that a system only has a probability of giving a particular result that really differentiates the quantum and classical worlds.

## 1.3 Dirac Notation

This thesis will **not** employ Dirac notation. Nevertheless, we shall for completeness, indicate here briefly how this Dirac notation is related to our more mathematical notation. This notation for abstract Hilbert spaces is extremely common among physicists and is also extremely convenient. However, its use does have a tendency to obscure some of the mathematics involved and some of the formal manipulations which it allows (and are commonly used) are mathematically suspect to say the least.

In Dirac notation, the vectors of a Hilbert space are denoted $|f\rangle$ corresponding to our $f$, and are called *ket* vectors. In addition, there are vectors denoted $\langle g|$ called *bra* vectors. These are multiplied together to give a *bra-ket* (bracket): $\langle g|\,f\rangle$. The bra-ket is of course analogous to our inner-product $\langle g, f\rangle$. To establish what the bra vectors correspond to, we recall theorem 3. Since any $\phi \in \mathscr{H}'$ satisfies $\phi(f) = \langle g, f\rangle$ for some $g \in \mathscr{H}$, we have that $\phi(f) \equiv \langle g|\,(|f\rangle) = \langle g|\,f\rangle \equiv \langle g, f\rangle$ so $\langle g|$ corresponds to the continuous linear functional in $\mathscr{H}'$ generated by $g$.

# Chapter 2

# Operator Theory

*"Mathematicians are like Frenchmen: Whatever you say to them they translate into their own language and forthwith it is something entirely different."*
Goethe

## 2.1 Properties and Classes of Operators

Many of the classes of operators which commonly occur in quantum mechanics also occur frequently in other areas of analysis and as such, are well known to mathematicians. The theory involved is thus well known. Therefore in this section, we shall state many simple facts regarding these classes of operators. Proofs may be found in the standard texts (eg [17], [21], [27], [42]).

### 2.1.1 Bounded Operators

We shall begin our study of operators with the important concept of continuity. We shall say that an operator, $A$, is *continuous* if $f_n \to f \Rightarrow Af_n \to Af$. We immediately note that if $A$ is bounded then $\|Af_n - Af\| \leqslant \|A\| \, \|f_n - f\| \to 0$ so $A$ is continuous. The converse is also true.

We shall however, be often discussing unbounded operators. As an example of an unbounded operator, we give the position operator $x$ acting in $L^2(\mathbb{R})$, defined by $(xf)(x) = xf(x)$. That is, multiplication by $x$. Define $f_n = \chi_{[n,n+1]}$, the characteristic function of $[n, n+1]$; so $\|f_n\| = 1$. Then,

$$\|xf_n\|^2 = \int_n^{n+1} x^2 dx \geqslant n^2 = n^2 \|f_n\|^2$$

so $\|x\| \geqslant n \quad \forall n$ and $x$ is unbounded.

### 2.1.2 Adjoints

In quantum theory the unboundedness of the position operator is unfortunately not an exception. Most operators we shall study in relation to quantum theory will be unbounded. This means that we do not always have continuity at our disposal but it does mean the theory is richer if much more difficult. In fact, the study of unbounded operators was catalysed by the development of quantum theory. A chief difficulty lies with the domain of an unbounded operator. We may define a bounded operator, $A$, acting on any vector $f \in \mathscr{H}$ without encountering problems since $A$ can only magnify the norm of $f$ by $\|A\|$ which is finite. Thus $Af$ has finite norm and is thus in $\mathscr{H}$. However, an unbounded operator has (loosely speaking) infinite norm and so $Af$ may not be in $\mathscr{H}$. Mathematically, we do not allow $A$ to act on such an $f$ and hence we must restrict the domain of an unbounded operator. For example, the domain of the position operator $\mathbf{x}$ is the set

$$\mathscr{D}_{\mathbf{x}} = \left\{ f(x) \in L^2(\mathbb{R}) : \int_{\mathbb{R}} x^2 |f(x)|^2 dx < \infty \right\}$$

which is a proper subset of $L^2(\mathbb{R})$ (The function $g(x) = x^{-1}$ when $|x| > 1$ and $g(x) = 1$ elsewhere is in $L^2(\mathbb{R})$ but not $\mathscr{D}_{\mathbf{x}}$).

We note that when $A$ is a bounded operator, densely defined in $\mathscr{H}$, it is easy to show using the continuity of $A$ that we can *extend* $A$ so that it is defined on all $\mathscr{H}$. Hence, when we speak of a (densely defined) bounded operator, we shall implicitly assume that it is defined on all of $\mathscr{H}$. Generally, we shall call $A'$ an *extension* of $A$ if $\mathscr{D}_{A'} \supseteq \mathscr{D}_A$ and $A'f = Af \quad \forall f \in \mathscr{D}_A$, and write $A' \supseteq A$.

We shall now define the adjoint $A^\dagger$ of an operator $A$ (bounded or unbounded) as follows. The domain of $A^\dagger$ is the set

$$\mathscr{D}_{A^\dagger} = \{g \in \mathscr{H} : \forall g, \quad \exists h \in \mathscr{H}, \text{ unique, such that } \langle h, f\rangle = \langle g, Af\rangle \quad \forall f \in \mathscr{D}_A\}$$

and we define $A^\dagger g = h$ on this set. With such a definition, the question of existence automatically arises and it turns out that $A^\dagger$ exists (in that $\mathscr{D}_{A^\dagger} \neq \varnothing$) iff $\mathscr{D}_A$ is dense in $\mathscr{H}$.

Note that if $A \subseteq B$ where $A$ is densely defined then $B^\dagger \subseteq A^\dagger$. It is not hard to show that if $A \in B(\mathscr{H})$ then $A^\dagger \in B(\mathscr{H})$ with $\|A\| = \left\|A^\dagger\right\|$. We also have that if $f \in \mathscr{D}_A$, and $g \in \mathscr{D}_{A^\dagger}$ (dense in $\mathscr{H}$), $\langle g, Af\rangle = \left\langle A^\dagger g, f\right\rangle = \left\langle g, A^{\dagger\dagger} f\right\rangle$ so $f \in \mathscr{D}_{A^{\dagger\dagger}}$ and $A^{\dagger\dagger} f = Af$. That is, $A^{\dagger\dagger} \supseteq A$ and so $A^{\dagger\dagger}$ is an extension of $A$. If in addition, $A \in B(\mathscr{H})$, then $\mathscr{D}_A = \mathscr{H}$ so $A^{\dagger\dagger} = A$.

A related concept (but much more important) is the idea of a *self-adjoint operator*. This is, naturally, an operator satisfying $A = A^\dagger$ (that is, $\mathscr{D}_A = \mathscr{D}_{A^\dagger}$ and $Af = A^\dagger f$ for all $f \in \mathscr{D}_A$). A similar but weaker concept is that of a *symmetric operator* which is required to satisfy $\langle g, Af\rangle = \langle Ag, f\rangle \quad \forall f, g \in \mathscr{D}_A$. An *unbounded* symmetric operator need not be self-adjoint since $A$ and $A^\dagger$ need only agree on $\mathscr{D}_A$. That is, $A \subseteq A^\dagger$. We shall discuss some symmetric operators which are not self-adjoint in chapter 3. As mentioned in Chapter 1, operators that correspond to observable quantities in quantum theory must be self-adjoint. This is because the expectation values have the form $\langle f, Af\rangle$ which are real numbers since $\langle f, Af\rangle = \langle Af, f\rangle = \overline{\langle f, Af\rangle}$. This however, holds for symmetric operators too. The requirement that the observables must be self-adjoint appears to be made because the spectral theorem (theorem 17) cannot be modified to include all symmetric operators [42]. This theorem lies at the heart of any Hilbert space formulation of quantum theory.

We shall finish this section with a very important result which uses the uniform boundedness principle. We also introduce the common phrasing: If $\mathscr{D}_A = \mathscr{H}$ then $A$ is said to be defined *on* $\mathscr{H}$ and otherwise, $A$ is said to be defined *in* $\mathscr{H}$.

**Lemma 6 (Uniform Boundedness Principle)** *Suppose $(\phi_n) \subseteq \mathscr{H}'$ is a sequence of continuous linear functionals on $\mathscr{H}$ for which $|\phi_n(f)| \leqslant c(f)$ for all $n$ where $c(f)$ are constants. Then, $\exists C > 0$ such that $|\phi_n(f)| \leqslant C\|f\|$.*

**Theorem 7 (Hellinger and Toeplitz)** *Any symmetric operator defined on $\mathscr{H}$ is bounded.*

**Proof.** Let $A$ be symmetric and defined on $\mathscr{H}$ so $A^\dagger$ is also defined on $\mathscr{H}$. If $A^\dagger$ is unbounded then $\exists (g_n) \subseteq \mathscr{H}$ such that $\|g_n\| = 1$ and $\left\|A^\dagger g_n\right\| \to \infty$. We may define $\phi_n(f) = \langle g_n, Af\rangle \quad \forall f \in \mathscr{H}$ and for any given $n$, so these functionals are bounded thus continuous. For fixed $f$ then, $|\phi_n(f)| \leqslant \|g_n\|\,\|Af\| = \|Af\| \equiv c(f)$. Therefore, by the uniform boundedness principle, $\exists C > 0$ such that $|\phi_n(f)| \leqslant C\|f\| \quad \forall f \in \mathscr{H}$. In particular, $\left|\phi_n\left(A^\dagger g_n\right)\right| = \left\|A^\dagger g_n\right\|^2 \leqslant C\left\|A^\dagger g_n\right\|$. Hence $\left\|A^\dagger g_n\right\|$ is uniformly bounded by $C$, contradicting unboundedness of $A^\dagger$. $A^\dagger$ is thus bounded and since $A$ is symmetric, $A = A^\dagger$ on $\mathscr{H}$ so $A$ is also bounded. ■

Thus we have proven that there are no unbounded self-adjoint operators defined on $\mathscr{H}$. Therefore in quantum theory, where unbounded operators abound (as it were), domain problems will be a common nuisance.

### 2.1.3 Projections

Let us consider a closed subspace $M$ of $\mathscr{H}$. Since $\mathscr{H} = M \oplus M^\perp$ (the *direct sum* of $M$ and $M^\perp$, its orthogonal complement) we can write $f = f' + f''$ for any $f \in \mathscr{H}$ where $f' \in M$ and

$f'' \in M^{\perp}$. We define the *projection operator* (*projector*) *onto* $M$ by $E_M f = f'$. An equivalent definition is that an operator $E \in B(\mathscr{H})$ is a projector if $E$ is self-adjoint and idempotent ($E^2 = E$). $E$ then projects onto the set $M = \{f \in \mathscr{H} : Ef = f\}$. We see immediately that provided $M \neq \{0\}$, $\|E_M\| = 1$. There are a number of other algebraic properties of projectors of interest which we list below.

**Theorem 8** *Let $E_M$ and $E_N$ be projectors onto closed subspaces $M$ and $N$ of $\mathscr{H}$ respectively. Then:*

$$\begin{aligned} M \perp N \text{ iff } E_M E_N &= 0, \\ E_M E_N \text{ is a projector, } E_{M\cap N}, \text{ iff } [E_M, E_N] &= 0, \\ E_M + E_N \text{ is a projector, } E_{M\oplus N}, \text{ iff } E_M E_N &= 0, \\ \sum_{i=1}^{\infty} E_{M_i} \text{ is a projector, } E_{\oplus_{i=1}^{\infty} M_i}, \text{ iff } E_{M_i} E_{M_j} &= 0 \quad \forall i, j. \end{aligned}$$

*where* $[A,B] = AB - BA$,.

We shall also find it convenient to introduce a *partial ordering* on projectors. We shall define $E_M \leqslant E_N$ when $M \subseteq N$.

### 2.1.4 Isometric and Unitary Operators

An *isometric operator* (or *isometry*), $U$, satisfies $\langle Uf, Ug\rangle = \langle f, g\rangle \quad \forall f, g \in \mathscr{H}$. If in addition the range of $U$ (denoted $\mathscr{R}_U$) is $\mathscr{H}$ then $U$ is a *unitary operator*. Equivalently, it is easy to show that $U$ is isometric iff $\|Uf\| = \|f\| \quad \forall f \in \mathscr{H}$. It obviously follows that $\|U\| = 1$. We shall also define the *left-inverse*, $U^{-1}$, of an operator $U$ by $U^{-1}U = I$ (the identity operator) where $\mathscr{D}_{U^{-1}} = \mathscr{R}_U$. $U^{-1}$ exists iff the equation $Uf = 0$ has the unique solution $f = 0$. We then have the important characterisation that $U \in B(\mathscr{H})$ is unitary iff $U^{\dagger} = U^{-1}$.

There is a useful link between unitary and self-adjoint operators - this is the *Cayley transform*. The Cayley transform of a symmetric operator $A$ is defined by $V = (A-i)(A+i)^{-1}$. This may also be inverted giving $A = i(1+V)(1-V)^{-1}$ and $\mathscr{D}_A = \mathscr{R}_{1-V}$. We note that $(A \pm i)^{-1}$ exists (as a left-inverse) since

$$\|(A \pm i) f\|^2 = \|Af\|^2 \pm i\langle Af, f\rangle \mp i\langle f, Af\rangle + \|f\|^2 = \|Af\|^2 + \|f\|^2 \tag{2.1}$$

so $(A \pm i) f = 0 \Rightarrow f = 0$. Furthermore, we have $\|(A-i) f\| = \|(A+i) f\|$ so taking $f = (A+i)^{-1} g$, for some $g \in \mathscr{R}_{A+i}$, gives $\left\|(A-i)(A+i)^{-1} g\right\| = \|g\|$. Thus, $V$ is isometric from $\mathscr{R}_{A+i}$ to $\mathscr{R}_{A-i}$. Of importance is the fact that we can do slightly better than this [38].

**Theorem 9** *Suppose $A$ is symmetric and densely defined. Then $A$ is self-adjoint iff its Cayley transform is unitary.*

It should be realised that even though $A$ may be unbounded and hence not everywhere defined, its Cayley transform is defined everywhere. That is, it is not just unitary on its domain of definition. We shall demonstrate this explicitly in section 3.2.1 with the position operator.

### 2.1.5 Closed Operators

We know that unbounded operators are not continuous. However, a weaker version of continuity is available. An operator $A$ in $\mathscr{H}$ is *closed* if given a sequence $(f_n) \subseteq \mathscr{D}_A$ satisfying $f_n \to f$ and $Af_n \to g$ for some $f, g \in \mathscr{H}$, we also have that $f \in \mathscr{D}_A$ and $g = Af$. Clearly $A$ is closed if $A$ is continuous. We also note that the adjoint of any operator is closed. We see this by taking $f_n \to f$ and $A^{\dagger} f_n \to g$ ($(f_n) \subseteq \mathscr{D}_{A^{\dagger}}$) and noting that if $h \in \mathscr{D}_A$, $\langle g, h\rangle = \lim_{n\to\infty} \langle A^{\dagger} f_n, h\rangle = \lim_{n\to\infty} \langle f_n, Ah\rangle = \langle f, Ah\rangle$ so $f \in \mathscr{D}_{A^{\dagger}}$ and $g = A^{\dagger} f$. We thus get the nice result that every self-adjoint unbounded operator is closed.

Let us now define the *closure* of an operator $A$ (when it exists) to be the closed operator $\overline{A}$ which is such that $\overline{A} \subseteq C$ where $C$ is any closed extension of $A$. $\overline{A}$ exists whenever $A$ has a closed extension. If $A$ is symmetric, $A^\dagger \supseteq A$, so $\overline{A}$ exists. In fact, the relationship between such an operator and its closure is simple [38]

**Theorem 10** *If $A$ is densely defined and symmetric then $\overline{A} = A^{\dagger\dagger}$.*

In the next chapter we will construct self-adjoint operators by closing symmetric operators.

## 2.2 Spectral Theory

The spectral theory of operators is the natural generalisation of the eigenvalue theory of matrices and is fundamental to quantum theory. It is not an easy theory, essentially because we shall be working with infinitely many dimensions, but it does facilitate much algebraic manipulation and gives insight into the behaviour of particular classes of operators. The ends will justify the means. Our primary concern here is the spectral decomposition of an unbounded self-adjoint operator as these are the most important in quantum mechanics. To do this, we shall follow the original method of Von Neumann.

### 2.2.1 Introduction - Finite Dimensions

We shall begin with a short preview of spectral theory by assuming that $\dim \mathscr{H} = n < \infty$. We shall decompose an operator $A$ using the familiar process of finding eigenvectors of a corresponding matrix. We define an *eigenvalue* of $A$ to be a complex scalar $\lambda$ which satisfies $Af = \lambda f$ for some $f \neq 0$. The vector $f$ is an *eigenvector* of $A$ corresponding to $\lambda$. The eigenvectors for a particular eigenvalue $\lambda$ span a subspace (or *eigenspace*) of $\mathscr{H}$ which we shall denote by $M_\lambda$, the set of eigenvalues we shall denote by $\sigma$.

Now, suppose that $A$ is self-adjoint. Therefore the eigenspaces of $A$ span $\mathscr{H}$ [29]. That is, $\mathscr{H} = \oplus_{\lambda\in\sigma} M_\lambda$. We can thus decompose any $f \in \mathscr{H}$ uniquely as $f = \sum_{\lambda\in\sigma} f_\lambda$ where $f_\lambda \in M_\lambda$. In fact, using the projection operators onto $M_\lambda$, which we shall denote by $E_{M_\lambda}$, we can write

$$\begin{aligned} Af &= A\sum_{\lambda\in\sigma} f_\lambda = \sum_{\lambda\in\sigma} Af_\lambda = \sum_{\lambda\in\sigma} \lambda f_\lambda = \sum_{\lambda\in\sigma} \lambda E_{M_\lambda} f \\ \Rightarrow\ A &= \sum_{\lambda\in\sigma} \lambda E_{M_\lambda}. \end{aligned}$$

We can be more transparent with respect to what will follow by ordering the eigenvalues, $\lambda_1, < \ldots <, \lambda_n$ and letting $E_{\lambda_k} = \sum_{\lambda\leqslant\lambda_k} E_{M_\lambda}$. The $E_{\lambda_k}$ are projectors by theorem 8 as the $M_\lambda$ are all orthogonal [27]. Then we can rewrite the decomposition in the form

$$A = \sum_{k=1}^{n} \lambda_k \left(E_{\lambda_k} - E_{\lambda_{k-1}}\right)$$

where $E_{\lambda_0} = 0$. This looks suspiciously similar to a Riemann approximation to the (symbolic) integral

$$A = \int \lambda dE_\lambda.$$

That this integral representation can be shown to hold (in a sense) in infinite dimensional Hilbert spaces is the important result that we shall derive in section 2.2.4 as the spectral theorem for self-adjoint operators.

### 2.2.2 Spectral Measures

It is apparent that if we were to try to write the decomposition of a self-adjoint operator over a finite dimensional Hilbert space as an integral then the family of projections $\{E_\lambda\}$ must be

in some sense stationary except when $\lambda = \lambda_k$, an eigenvalue, when $E_\lambda$ 'increases' in a discontinuous fashion. This is most readily seen in the formula $E_\lambda = \sum_{\mu \leqslant \lambda} E_{M_\mu}$ from the previous section where it is easy to see that $E_\mu \leqslant E_\lambda$ (partial ordering on projectors) if $\mu \leqslant \lambda$. The same idea will form the starting point for the general treatment of infinite dimensional spaces. This type of generalisation is necessary because we shall encounter the added complication that eigenvalues are not the only points at which $E_\lambda$ can increase.

We shall define abstractly a *spectral function* (*spectral family*) to be a function $E_\lambda$ defined for all $\lambda \in \mathbb{R}$ which takes projection operators as its values and satisfies

$$\begin{aligned} E_\mu &\leqslant E_\lambda \text{ whenever } \mu \leqslant \lambda, \\ E_\lambda &= \mathrm{s}-\lim_{\mu \to \lambda^+} E_\mu, \\ E_{-\infty} &= \mathrm{s}-\lim_{\mu \to -\infty} E_\mu = 0 \text{ and } E_\infty = \mathrm{s}-\lim_{\mu \to \infty} E_\mu = I \end{aligned}$$

where 0 is the zero operator and $I$ is the identity operator.

Similarly, we shall define a *spectral measure* to be a projector-valued function defined on a collection of subsets of $\mathbb{R}$ satisfying

$$\begin{aligned} E(\mathbb{R}) &= I \\ \text{and } E\left(\bigcup_{k=1}^{\infty} B_k\right) &= \sum_{k=1}^{\infty} E(B_k) = \mathrm{s}-\lim_{n \to \infty} \sum_{k=1}^{n} E(B_k) \end{aligned}$$

for any countable sequence $(B_k)$ of disjoint subsets of $\mathbb{R}$. For any spectral measure then, we have $E(\emptyset) = 0$ and $E(B_1)E(B_2) = E(B_1 \cap B_2)$ [17]. Furthermore it can be shown that any spectral measure $E(B)$ generates a unique spectral function $E_\lambda$ and conversely, through the correspondence [38]

$$E_\lambda = E((-\infty, \lambda]).$$

All of these results may be generalised predictably from functions over $\mathbb{R}$ to functions over $\mathbb{R}^n$.

### 2.2.3 Spectral Theorem for Unitary Operators

Although we are primarily concerned with the decomposition of an unbounded self-adjoint operator, we shall derive this from the decomposition of a unitary operator which is bounded and hence more tractable. Other derivations may be found in [17] and [42].

We begin with a topological lemma, proved in [20]. We shall also need to define the important concept of positivity as it applies to symmetric operators. A symmetric operator $A$ is *positive* if $\langle f, Af \rangle \geqslant 0$ for every $f \in \mathscr{D}_A$. This concept induces a partial ordering on the set of bounded self-adjoint operators: we write $A \geqslant B$ if $A - B$ is positive.

**Lemma 11** *Suppose we have a monotonically decreasing sequence of bounded positive self-adjoint operators ($A_1 \geqslant A_2 \geqslant A_3 \geqslant \ldots$). Then $A_n$ converges strongly to a bounded self-adjoint operator $A$.*

Let $U$ be a unitary operator. Since $\|U\| = 1$, we shall associate it with the function $e^{i\theta}$ which has modulus one. This may be conveniently achieved by constructing a transformation taking the trigonometric polynomials into $B(\mathscr{H})$. Specifically, we map $p\left(e^{i\theta}\right) = \sum_{k=-n}^{n} c_k e^{ik\theta}$ to $\sum_{k=-n}^{n} c_k U^k = p(U)$. It is easy to see that the mapping is linear, that $p\left(e^{i\theta}\right) q\left(e^{i\theta}\right)$ is mapped to $p(U)q(U)$, and that $\overline{p\left(e^{i\theta}\right)}$ is mapped to $[p(U)]^\dagger$. Our mapping is therefore a type of $*$-*homomorphism*. The mapping also preserves positivity since if $p\left(e^{i\theta}\right) \geqslant 0$ then by Fejer's lemma [48], $p\left(e^{i\theta}\right) = \left|q\left(e^{i\theta}\right)\right|^2$ for some trigonometric polynomial $q$. Thus $p(U) = [q(U)]^\dagger q(U)$ and $\langle f, p(U) f \rangle = \langle q(U) f, q(U) f \rangle \geqslant 0$, so $p(U)$ is positive. We now invoke lemma 11 to extend this mapping to the set $\mathfrak{T}$ of all functions which are the pointwise limits of sequences of monotonically decreasing positive trigonometric polynomials.

**Lemma 12** *Suppose that $(p_n)$ is a sequence of monotonically decreasing positive trigonometric polynomials so that $u(\theta) = \lim_{n\to\infty} p_n\left(e^{i\theta}\right) \in \mathfrak{T}$. Then there exists a positive symmetric operator $A \in B(\mathscr{H})$ such that $p_n(U) \to A$ strongly and $A$ is independent of the choice of sequence $(p_n)$.*

**Proof.** Since $(p_n)$ is monotonically decreasing and bounded below by 0, lemma 11 guarantees existence of $A$. Also $\langle f, Af\rangle = \mathrm{w}-\lim_{n\to\infty} \langle f, p_n(U) f\rangle \geqslant 0$, so $A$ is positive. Furthermore, if $\lim_{n\to\infty} p_n^{(1)}\left(e^{i\theta}\right) = \lim_{n\to\infty} p_n^{(2)}\left(e^{i\theta}\right)$ everywhere then given an $n$, $\exists k$ such that $p_k^{(1)}\left(e^{i\theta}\right) \leqslant p_n^{(2)}\left(e^{i\theta}\right) + 1/n$, since both sequences are monotonically decreasing. Thus $p_k^{(1)}(U) \leqslant p_n^{(2)}(U) + 1/n$, so $\mathrm{s}-\lim_{n\to\infty} p_n^{(1)}(U) \leqslant \mathrm{s}-\lim_{n\to\infty} p_n^{(2)}(U)$. The opposite inequality is obtained similarly. Hence $A$ is independent of $(p_n)$. ■

This lemma is extremely important as it allows us to work with the limits of trigonometric polynomials. In particular, we should like to apply the result to functions $\chi$ which would give a projector under our mapping. Since projectors are idempotent, we require our function to satisfy $\chi(\theta) = [\chi(\theta)]^2$ everywhere. Thus $\chi$ is a characteristic function. This also requires $\chi$ to be real-valued, so the mapping will give a self-adjoint operator, just what we want of a projector. These projectors will be used to construct a spectral function for $U$.

Since we are taking pointwise limits of $2\pi$-periodic trigonometric functions, the characteristic functions we employ must also be $2\pi$-periodic. Also, we have seen that spectral functions and spectral measures are related on $\mathbb{R}$ by $E_\lambda = E((-\infty, \lambda])$ where $E_{-\infty} = 0$ and $E_\infty = I$. Thus, on $[0, 2\pi]$, we shall use characteristic functions of the interval $(0, \lambda]$. More concretely, we shall define a family of $2\pi$-periodic functions $\Omega_\lambda$ by

$$\begin{aligned} \Omega_\lambda(\theta) &= 0 \text{ when } \lambda \leqslant 0, \\ \Omega_\lambda(\theta) &= 1 \text{ when } \lambda \geqslant 2\pi \\ \text{and } \Omega_\lambda(\theta) &= \chi_{(0,\lambda]}(\theta) \text{ for } 0 < \lambda < 2\pi,\ 0 \leqslant \theta < 2\pi. \end{aligned}$$

We now show that $\Omega_\lambda \in \mathfrak{T}$ by taking a strictly decreasing sequence of continuous differentiable functions $(g_n)$ which converge to $\Omega_\lambda$ pointwise and satisfy $g_{n+1}(\theta) < g_n(\theta) - \delta_n$ everywhere (where $\delta_n > 0$). That is, there is a non-vanishing 'gap' between any two of the $g_n$. Each of these can then be approximated uniformly by a sequence of trigonometric polynomials $p_{n,m}(\theta)$ [38] and because of the 'gap' between the $g_n$, we can choose for each $n$, a $p_{n,k_n}$ such that the $p_{n,k_n}(\theta)$ are also strictly decreasing everywhere. Clearly this sequence of trigonometric polynomials must converge pointwise to $\Omega_\lambda$ so $\Omega_\lambda \in \mathfrak{T}$.

The projectors corresponding to $\Omega_\lambda$ shall of course be denoted by $E_\lambda$. It remains then to prove that these projectors do in fact constitute a spectral function and to show how this spectral function is related to our original unitary operator $U$.

**Theorem 13 (Spectral Theorem for a Unitary Operator)** *The $E_\lambda$ defined above constitute a spectral function with which $U$ may be written*

$$U = \int_0^{2\pi} e^{i\lambda}\, dE_\lambda.$$

***Proof.*** *The last requirement (see definition) is apparent from the construction. The first is seen by noting that if $\mu \leqslant \lambda$, $\Omega_\mu(\theta)\Omega_\lambda(\theta) = \Omega_\mu(\theta)$ which maps to $E_\mu E_\lambda = E_\mu$, hence $E_\mu \leqslant E_\lambda$. We thus need only show that $E_\lambda = s-\lim_{\mu\to\lambda^+} E_\mu$. Consider a monotonically decreasing sequence of trigonometric polynomials $(p_n)$ which converge to $\Omega_\lambda$ pointwise but for which $p_n\left(e^{i\theta}\right) \geqslant \Omega_{\lambda+1/n}(\theta)$ for all $n$. Thus $p_n(U) \geqslant E_{\lambda+1/n}$. However, since $E_\lambda \leqslant E_{\lambda+1/n}$,*

$$E_\lambda \leqslant s-\lim_{n\to\infty} E_{\lambda+1/n} \leqslant s-\lim_{n\to\infty} p_n(U) = E_\lambda,$$

*so we have $E_\lambda = s-\lim_{n\to\infty} E_{\lambda+1/n}$. Since for any sequence converging to 0 from above, there is a subsequence of $(1/n)$ which converges faster, the second requirement is met so $E_\lambda$ is a spectral*

*function.*
*Now, since* $E_\lambda = 0$ *when* $\lambda \leqslant 0$ *and* $E_\lambda = I$ *when* $\lambda \geqslant 2\pi$, $E_\lambda$ *is only increasing on* $[0,2\pi]$. *Let us partition this interval into* $0 = \lambda_0 < \lambda_1 < \ldots < \lambda_{n-1} < \lambda_n = 2\pi$ *and choose* $\lambda_k'$ *such that* $\lambda_{k-1} < \lambda_k' \leqslant \lambda_k$ *for* $k = 1,\ldots,n$. *If we let* $\phi \in [\lambda_{k-1},\lambda_k]$, *then* $\Omega_{\lambda_\ell}(\phi) - \Omega_{\lambda_{\ell-1}}(\phi) = \delta_{k\ell}$ *(*1 *if* $k = \ell$ *and* 0 *otherwise) so if* $\varepsilon = \max(\lambda_k - \lambda_{k-1})$,

$$\left| e^{i\phi} - \sum_{\ell=1}^{n} e^{i\lambda_\ell'} \left[ \Omega_{\lambda_\ell}(\phi) - \Omega_{\lambda_{\ell-1}}(\phi) \right] \right| \leqslant \left| e^{i\phi} - e^{i\lambda_k'} \right| \leqslant \left| \phi - \lambda_k' \right| \leqslant \varepsilon$$

*by the mean value theorem. Since this holds for any k we have for any* $\theta \in [0,2\pi]$,

$$\left| e^{i\theta} - \sum_{k=1}^{n} e^{i\lambda_k'} \left[ \Omega_{\lambda_k}(\theta) - \Omega_{\lambda_{k-1}}(\theta) \right] \right|^2 \leqslant \varepsilon^2.$$

*Writing this as a function multiplied by its conjugate and then applying our familiar mapping gives*

$$V^\dagger V \leqslant \varepsilon^2 I \text{ where } V = U - \sum_{k=1}^{n} e^{i\lambda_k'} \left[ E_{\lambda_k} - E_{\lambda_{k-1}} \right].$$

*That is,*

$$\|Vf\|^2 = \langle f, V^\dagger V f \rangle \leqslant \varepsilon^2 \|f\|^2 \text{ so } \|V\| = \left\| U - \sum_{k=1}^{n} e^{i\lambda_k'} \left[ E_{\lambda_k} - E_{\lambda_{k-1}} \right] \right\| \leqslant \varepsilon.$$

*If we now insist that* $\varepsilon = \max(\lambda_k - \lambda_{k-1}) \to 0$, *then n must necessarily go to* $\infty$ *giving*

$$U = u - \lim_{\varepsilon \to 0} \sum_{k=1}^{n} e^{i\lambda_k'} \left[ E_{\lambda_k} - E_{\lambda_{k-1}} \right] \equiv \int_0^{2\pi} e^{i\lambda} dE_\lambda.$$

■

We have essentially defined the *spectral integral* appearing in the previous theorem by the uniform limit of a Riemann sum of operators. Although the operators $E_\lambda$ induce a spectral measure $E(B)$ on $\mathbb{R}$, this is clearly not a measure in the usual sense (being operator-valued). It is therefore not obvious that the usual results applying to integration are valid. However, it is easy to construct a bona-fide measure from a spectral measure and we shall do so shortly.

Let us first define a *complex measure* on $\mathbb{R}$ to be a finite linear combination of finite measures on $\mathbb{R}$, a finite measure on $\mathbb{R}$ being a measure $\nu$ satisfying $\nu(\mathbb{R}) < \infty$. It is easy to see that since integration is linear, results holding for integration with respect to a measure will also hold with respect to a complex measure.

We choose $f, g \in \mathscr{H}$ and take a spectral measure $E(B)$. Let $\mu_{f,g}(B) = \langle f, E(B) g \rangle$. It is easy to see that any function of the form $\nu(B) = \langle f, E(B) f \rangle$ is a finite measure on $\mathbb{R}$ since projections are positive. However, one can use the *parallelogram identity* [27] to write $\langle f, E(B) g \rangle$ as the sum of measures of the form $\nu(B)$. Therefore, $\langle f, E(B) g \rangle$ is a complex measure.

Now, since uniform convergence implies weak convergence, we can restate the last result in terms of the weak topology as follows:

$$\langle f, Ug \rangle = \lim_{\varepsilon \to 0} \sum_{k=1}^{n} e^{i\lambda_k'} \left\langle f, \left[ E_{\lambda_k} - E_{\lambda_{k-1}} \right] g \right\rangle \equiv \int_0^{2\pi} e^{i\lambda} d\langle f, E_\lambda g \rangle = \int_{\mathbb{R}} e^{i\lambda} d\mu_{f,g}((0,\lambda]).$$

The spectral integral may now be recognised in the weak topology as an ordinary *Riemann-Stieltjes* integral and as such, general measure theory results such as the Dominated Convergence theorem can be applied. We shall use this to prove the following.

**Theorem 14** *The spectral function of a unitary operator is unique.*

**Proof.** Suppose that $E_\lambda$ and $F_\lambda$ are both spectral families for $U$, unitary. It is easy to check using the decomposition $U = \mathrm{u}-\lim_{\varepsilon\to 0}\sum_{k=1}^{n} e^{i\lambda_k'}\left[F_{\lambda_k} - F_{\lambda_{k-1}}\right]$ and the orthogonality of the projections $\left[F_{\lambda_k} - F_{\lambda_{k-1}}\right]$ $(k = 1,\ldots,n)$ that

$$p(U) = \int_0^{2\pi} p\left(e^{i\lambda}\right) dF_\lambda \quad \text{and} \quad \langle f, p(U) g\rangle = \int_0^{2\pi} p\left(e^{i\lambda}\right) d\langle f, F_\lambda g\rangle$$

hold for any trigonometric polynomial $p\left(e^{i\lambda}\right)$. Now, $\Omega_\psi(\lambda)$ as defined previously is the pointwise limit of a monotonically decreasing sequence of positive trigonometric functions so by dominated convergence,

$$\int_0^{2\pi} \Omega_\psi(\lambda)\, d\langle f, F_\lambda g\rangle = \lim_{n\to\infty}\int_0^{2\pi} p_n\left(e^{i\lambda}\right) d\langle f, F_\lambda g\rangle = \lim_{n\to\infty}\langle f, p_n(U) g\rangle = \left\langle f, E_\psi g\right\rangle$$

$$\Rightarrow \left\langle f, E_\psi g\right\rangle = \int_0^{\psi} d\langle f, F_\lambda g\rangle = \left\langle f, F_\psi g\right\rangle - \langle f, F_0 g\rangle = \left\langle f, F_\psi g\right\rangle.$$

Since this holds for any $f, g \in \mathscr{H}$, $E_\psi = F_\psi$ for all $\psi$ so the spectral function is unique. ■

### 2.2.4 Spectral Theorem for Self-Adjoint Operators

We have shown that a unitary operator $U$ on $\mathbb{R}$ can be decomposed using the unique spectral function $E_\lambda$ associated with $U$. We shall now show that a similar result holds for arbitrary (possibly unbounded) self-adjoint operators. This will be achieved by relating the self-adjoint operator to a unitary one by means of the Cayley transform (theorem 9). We shall need the following lemmas. The first is proven in [34].

**Lemma 15** *Let $\mu$ be a measure on $\mathbb{R}$ and let $\nu(S) = \int_S g d\mu$ for some fixed measurable function $g$ and any measurable subset $S$. Then $\nu$ is also a measure over $\mathbb{R}$ and $\int_B f d\nu = \int_B f g d\mu$ for any measurable function $f$ and measurable subset $B$.*

**Lemma 16** *If $F_\phi$ is the spectral function associated with a unitary operator $U$ then $UF_\phi = F_\phi U$ for all $\phi$.*

**Proof.** Choose $\phi$. For each $n > 0$, let us choose a partition of $[0, 2\pi]$ as in the proof of theorem 13 such that $\max\left|\lambda_k^{(n)} - \lambda_{k-1}^{(n)}\right| < 1/n$. We define

$$U_n = \sum_{k=1}^{n} e^{i\lambda_k^{(n)\prime}}\left(F_{\lambda_k^{(n)}} - F_{\lambda_{k-1}^{(n)}}\right)$$

so by theorem 13, $U_n \to U$ uniformly. Since the $F_{\lambda_k^{(n)}}$ commute with $F_\phi$, we have $U_n F_\phi = F_\phi U_n$ for all $n$. But, the separate multiplication of operators is continuous in the uniform topology [20] so $U_n F_\phi \to U F_\phi$ and $F_\phi U_n \to F_\phi U$. Therefore, by uniqueness of limits, $UF_\phi = F_\phi U$. ■

**Theorem 17 (Spectral Theorem for a Self-Adjoint Operator)** *If $A$ is a self-adjoint operator in $\mathscr{H}$ then there is a spectral function $E_\lambda$, $\lambda \in \mathbb{R}$ such that*

$$\langle f, Ag\rangle = \int_{\mathbb{R}} \lambda\, d\langle f, E_\lambda g\rangle$$

*for all $f \in \mathscr{H}$ and $g \in \mathscr{D}_A$.*

**Proof.** Since $A$ is self-adjoint, its Cayley transform $V$ is unitary. Let $F_\phi$ be the unique spectral function associated with $V$ and $F(B)$ the corresponding spectral measure so $V = \int_0^{2\pi} e^{i\phi} dF_\phi$. Now, if $g \in \mathscr{D}_A$, $Ag = i(1+V)h$ where $h = (1-V)^{-1} g$. We have then,

$$\begin{aligned}
\langle f, Ag\rangle &= i\langle f, h\rangle + i\langle f, Vh\rangle = i\int_0^{2\pi} d\left\langle f, F_\phi h\right\rangle + i\int_0^{2\pi} e^{i\phi} d\left\langle f, F_\phi h\right\rangle \\
&= i\int_0^{2\pi}\left(1 + e^{i\phi}\right) d\left\langle f, F_\phi h\right\rangle = \int_0^{2\pi}\left(-\cot\frac{\phi}{2}\right)\left(1 - e^{i\phi}\right) d\left\langle f, F_\phi h\right\rangle \\
&= \int_0^{2\pi}\left(-\cot\frac{\phi}{2}\right) d\nu_{f,h}((0,\phi]) \qquad (2.2)
\end{aligned}$$

where we have used lemma 15 in letting

$$\nu_{f,h}(B) = \int_B \left(1 - e^{i\phi}\right) d\left\langle f, F\left((0,\phi]\right) h\right\rangle .$$

However, we derive from lemma 16 and $g = (1-V)h$ that

$$\begin{aligned}
\langle f, F(B) g\rangle &= \langle f, F(B) h\rangle - \langle f, F(B) V h\rangle = \langle f, F(B) h\rangle - \langle f, VF(B) h\rangle \\
&= \int_0^{2\pi} d\left\langle f, F_\phi F(B) h\right\rangle - \int_0^{2\pi} e^{i\phi} d\left\langle f, F_\phi F(B) h\right\rangle \\
&= \int_0^{2\pi} \left(1 - e^{i\phi}\right) d\left\langle f, F_\phi F(B) h\right\rangle
\end{aligned}$$

and since $F_\phi F(B) = F\left((0,\phi]\right) F(B) = F\left((0,\phi] \cap B\right)$ [17], this becomes

$$\langle f, F(B) g\rangle = \int_B \left(1 - e^{i\phi}\right) d\left\langle f, F_\phi h\right\rangle = \nu_{f,h}(B) .$$

Substituting this into equation 2.2 then gives

$$\begin{aligned}
\langle f, Ag\rangle &= \int_0^{2\pi} \left(-\cot\frac{\phi}{2}\right) d\nu_{f,h}\left((0,\phi]\right) = \int_0^{2\pi} \left(-\cot\frac{\phi}{2}\right) d\left\langle f, F\left((0,\phi]\right) g\right\rangle \\
&= \int_0^{2\pi} \left(-\cot\frac{\phi}{2}\right) d\left\langle f, F_\phi g\right\rangle = \int_{\mathbb{R}} \lambda d\left\langle f, E_\lambda g\right\rangle
\end{aligned}$$

where we make the substitution $\lambda = -\cot(\phi/2)$ so $E_\lambda = F_{-2\cot^{-1}\lambda} = F_\phi$. ■

This is the spectral decomposition of an arbitrary self-adjoint operator. The spectral function $E_\lambda$ is clearly unique since $F_\phi$ is unique and may be increasing on the entire real axis. It is also apparent that this theorem only guarantees that the decomposition holds in the weak topology. We cannot expect the corresponding decomposition to hold for an unbounded self-adjoint operator in the uniform topology since any partial sum must necessarily have finite operator norm (being a linear combination of projectors). Uniform convergence is however achieved for bounded self-adjoint operators [42].

## 2.3 Functional Calculus

When proving the spectral theorem for unitary operators we defined polynomial functions of operators and extended this idea to the set of functions $\mathfrak{T}$ which are pointwise limits of monotonically decreasing sequences of trigonometric polynomials. One immediate advantage of having a spectral decomposition at hand is that it enables us to extend this idea again and discuss a much larger range of functions of operators. In fact, we shall also find it necessary to discuss functions of several operators. When these operator functions exist and have the desired properties is discussed below.

### 2.3.1 Compatible Operators

Let us suppose that we have two self-adjoint operators $A_1$ and $A_2$ with spectral measures $E^{A_1}(B_1)$ and $E^{A_2}(B_2)$ respectively. We say that $A_1$ and $A_2$ are *compatible* if the observables that they correspond to may be simultaneously measured to arbitrary accuracy. The Heisenberg Uncertainty Principle and its generalisations ([4] or [46]) state that this simultaneous measurement of observables is only possible if the operators corresponding to the observables commute. That is, $A_1$ and $A_2$ are *compatible iff* $A_1$ and $A_2$ commute. Therefore, Heisenberg's Uncertainty Principle states that the position and momentum operators (section 3.2) are incompatible. However, we must be careful when defining the commutant of unbounded self-adjoint operators as the operator $A_1A_2 - A_2A_1$ may only be defined on $\{0\}$. An alternative definition which reduces to the usual one for bounded operators [38] is that $A_1$ and $A_2$ commute if their

spectral measures commute. If $E^{A_1}(B_1)$ and $E^{A_2}(B_2)$ commute then $E^{A_1}(B_1)E^{A_2}(B_2)$ is also a projector-valued function on $\mathbb{R}^2$ and it is not hard to see that this also meets the requirements of a spectral measure. Just as $E^{A_1}(B_1)$ is associated with the operator $A_1$, it is natural to associate the spectral measure $E^{A_1}(B_1)E^{A_2}(B_2)$ with functions of $A_1$ and $A_2$. The point is that the theory we shall outline below only allows us to define functions of compatible operators. We cannot define a spectral measure for functions of incompatible operators as we have done above because then $E^{A_1}(B_1)E^{A_2}(B_2)$ may not be projector-valued.

### 2.3.2 Functions of Compatible Operators

Let us suppose that we have two compatible self-adjoint operators $A_1$ and $A_2$ with spectral measures $E^{A_1}(B_1)$ and $E^{A_2}(B_2)$ respectively. We shall denote by $E(B)$ the spectral measure on $\mathbb{R}^2$, $E(B_1 \times B_2) = E^{A_1}(B_1)E^{A_2}(B_2)$. If $p(\lambda_1,\lambda_2)$ is a measurable function on $\mathbb{R}^2$ which is bounded by $M$ say, then we can form the functional

$$\phi(f,g) = \int_{\mathbb{R}^2} p(\lambda_1,\lambda_2)\, d\langle f, E_{\lambda_1,\lambda_2} g\rangle$$

where $E_{\lambda_1,\lambda_2}$ is the spectral function associated with the spectral measure $E(B)$. This functional is defined for any $f,g \in \mathscr{H}$ since

$$\int_{\mathbb{R}^2} p(\lambda_1,\lambda_2)\, d\langle f, E_{\lambda_1,\lambda_2} g\rangle \leqslant \int_{\mathbb{R}^2} M d\langle f, E_{\lambda_1,\lambda_2} g\rangle = M\langle f,g\rangle$$

so $\phi$ is bounded. It is easily verified that $\phi$ is a sesquilinear functional on $\mathscr{H}\times\mathscr{H}$. Hence we can use the Riesz representation theorem to infer that there exists a bounded operator which we shall denote by $p(A_1,A_2)$ satisfying

$$\phi(f,g) = \langle f, p(A_1,A_2)\, g\rangle = \int_{\mathbb{R}^2} p(\lambda_1,\lambda_2)\, d\langle f, E_{\lambda_1,\lambda_2} g\rangle .$$

**Theorem 18 (The Functional Calculus)** *Let $p(\lambda_1,\lambda_2)$ and $q(\lambda_1,\lambda_2)$ be bounded measurable functions on $\mathbb{R}^2$ and let $A_1$ and $A_2$ be self-adjoint operators. Then, for any $c \in \mathbb{C}$,*

$$\begin{aligned} (cp)(A_1,A_2) &= cp(A_1,A_2), \\ (p+q)(A_1,A_2) &= p(A_1,A_2)+q(A_1,A_2), \\ \overline{p}(A_1,A_2) &= [p(A_1,A_2)]^\dagger \\ \textit{and } (pq)(A_1,A_2) &= p(A_1,A_2)\,q(A_1,A_2). \end{aligned}$$

*That is, this mapping from the set of bounded measurable functions to $B(\mathscr{H})$ is a $*$-homomorphism.*

The proof of this theorem is based on theorem 17 and the usual properties of integration [42]. This theorem also proves that any two functions of the compatible operators $A_1$ and $A_2$ must commute since the ordinary functions obviously commute. It is also clear that any function of the operators must also commute with the spectral measure.

It is also possible to extend the functional calculus further to encompass unbounded functions [42]. The only complication here is that because the functions themselves are unbounded, the operator functions will be unbounded in operator norm. Hence, domain questions are a nuisance.

**Theorem 19** *Let $p(\lambda_1,\lambda_2)$ and $q(\lambda_1,\lambda_2)$ be measurable functions on $\mathbb{R}^2$ and let $A_1$ and $A_2$ be self-adjoint operators. Then, for any $c \in \mathbb{C}$,*

$$\begin{aligned} (cp)(A_1,A_2) &= cp(A_1,A_2), \\ (p+q)(A_1,A_2) &\supseteq p(A_1,A_2)+q(A_1,A_2), \\ \overline{p}(A_1,A_2) &= [p(A_1,A_2)]^\dagger \textit{ if } p(A_1,A_2) \textit{ is densely defined,} \\ (pq)(A_1,A_2) &\supseteq p(A_1,A_2)\,q(A_1,A_2) \\ \textit{and } (p^n)(A_1,A_2) &= [p(A_1,A_2)]^n \textit{ for all integers } n. \end{aligned}$$

Furthermore, since $f \in \mathscr{D}_{p(A_1,A_2)}$ iff $\|p(A_1,A_2)\, f\| < \infty$, we can write the domain of $p(A_1,A_2)$ as the set of $f \in \mathscr{H}$ such that $\int_{\mathbb{R}^2} |p(\lambda_1,\lambda_2)|^2\, d\langle f, E_{\lambda_1,\lambda_2} f\rangle < \infty$.

## 2.4 The Spectrum and the Resolvent

We shall now define the *spectrum* of a (possibly unbounded) self-adjoint operator $A$ to be the set of $\lambda \in \mathbb{R}$ such that $A-\lambda$ has no bounded inverse. This definition is also valid for arbitrary operators. The spectrum of $A$ shall be denoted by $\sigma(A)$. We say that an operator $A$ is *bounded below* if there is an $\varepsilon > 0$ such that $\|Af\| \geqslant \varepsilon \|f\|$ for every $f \in \mathscr{D}_A$. Therefore, $\lambda \in \sigma(A)$ when $A-\lambda$ is not bounded below. In fact, for self-adjoint operators, this is the only way that $A-\lambda$ can have no bounded inverse [17].

So, given $\lambda \in \sigma(A)$, $A-\lambda$ is not bounded below so there exists a sequence of vectors $(f_n)$ such that $(A-\lambda) f_n \to 0$ but $f_n \nrightarrow 0$. We shall distinguish two cases. First, if there actually exists an $f \neq 0$ such that $(A-\lambda) f = 0$ then we say that $\lambda$ is in the *point spectrum* of $A$, denoted by $\sigma_p(A)$. In this case, $\lambda$ is an *eigenvalue* of $A$ and since $A-\lambda$ is not $1:1$, its inverse does not exist. Second, if there does not exist such an $f$ then $A-\lambda$ is $1:1$ so $(A-\lambda)^{-1}$ does exist (as a left inverse). However, then there exists a sequence $g_n = (A-\lambda) f_n$ such that $g_n \to 0$ but $(A-\lambda)^{-1} g_n = f_n \nrightarrow 0$. Thus, $(A-\lambda)^{-1}$ is an unbounded operator and $\lambda$ is said to be in the *continuous spectrum* of $A$, denoted by $\sigma_c(A)$.

There is an equivalent definition for a self-adjoint operator $A$ with spectral measure $E(B)$ [38] which is that the spectrum is the set:

$$\sigma(A) = \{\lambda \in \mathbb{R} : E((\lambda-\delta, \lambda+\varepsilon)) \neq 0 \quad \forall \delta, \varepsilon > 0\}.$$

That is, the set of all values $\lambda$ for which $E_\lambda$ is increasing on any open interval containing $\lambda$. The spectrum is then the support of the spectral measure. The point spectrum and the continuous spectrum are then defined as the sets

$$\sigma_p(A) = \{\lambda \in \mathbb{R} : E(\{\lambda\}) \neq 0\} \text{ and } \sigma_c(A) = \sigma(A) \setminus \sigma_p(A).$$

This definition, whilst not so elegant as the first (which is also more general), does facilitate the physical interpretation of the spectrum of a self-adjoint operator.

The spectrum of a self-adjoint operators physically represents all the possible values that one could get for the corresponding observable when making a measurement of the system. To see this, recall that the probability that a measurement of the observable corresponding to $A$ lies within a set $B$ is given by $\|\Psi\|^{-2} \langle \Psi, E(B)\Psi \rangle$ where $\Psi$ is the quantum state of the system (section 1.2.6). Therefore, if $B \cap \sigma(A) = \varnothing$ then by the second definition, the probability that the measurement is in $B$ is zero.

# Chapter 3

# The Operators of Quantum Theory

*"A mathematician may say anything he pleases but a physicist must be at least partially sane."*
J W Gibbs

## 3.1 The Fourier Transform Revisited

Let us now discuss the Fourier transform in more detail. For notational simplicity, we shall work with just one dimension - the generalisations to $n$ dimensions are immediate. Recall that in section 1.2.4 we defined the Fourier transform of a rapidly decreasing function $f \in S(\mathbb{R})$ by

$$\widehat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x) e^{-ikx} dx \tag{3.1}$$

the inverse Fourier transform of $\widehat{f} \in S(\mathbb{R})$ by

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \widehat{f}(k) e^{ikx} dk \tag{3.2}$$

and the Fourier operator $F$ on $S(\mathbb{R})$ by $F f = \widehat{f}$. We shall now extend this definition. It should also be noted that for complete generality, we should define

$$\widehat{f}(k) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} f(x) e^{-ikx/\hbar} dx$$

where $\hbar$ is Planck's constant divided by $2\pi$. However, it is common practice in theoretical physics to work with units in which $\hbar = 1$, thus simplifying the equations. This implicit assumption of course validates our definition and brings it into line with the familiar mathematical one.

Since any $f \in S(\mathbb{R})$ is bounded and decays rapidly, $f$ must be square-integrable also. That is, $S(\mathbb{R}) \subseteq L^2(\mathbb{R})$. Furthermore, it is easy to see that all functions of the form $p(x) e^{-\alpha x^2}$, $\alpha > 0$, are of rapid decrease. Since these include the *Hermite functions* which form an orthonormal basis of $L^2(\mathbb{R})$ [27], we can conclude that $S(\mathbb{R})$ must be dense in $L^2(\mathbb{R})$.

It is also well known that for any $f \in S(\mathbb{R})$, *Parseval's equality* holds:

$$\int_{\mathbb{R}} |f(x)|^2 dx = \int_{\mathbb{R}} \left|\widehat{f}(k)\right|^2 dk.$$

In terms of the $L^2$-norm, this is $\|f\| = \left\|\widehat{f}\right\| = \|Ff\|$, so the Fourier operator $F$ is isometric on $S(\mathbb{R})$. In fact, since the Fourier transform and the inverse Fourier transform are indeed inverses on the space $S(\mathbb{R})$ [40], $F$ maps $S(\mathbb{R})$ onto $S(\mathbb{R})$. Therefore, $F$ is unitary. Thus $F$ is bounded and densely defined and so may be uniquely extended (section 2.1.2) to an operator defined on all of $L^2(\mathbb{R})$ which by continuity, must be isometric. This operator we shall denote by $U_F$. That this extension is in fact a unitary operator follows from the next lemma.

**Lemma 20** *If $W$ is dense in a Hilbert space $\mathscr{H}$ and its image $\widehat{W} = A(W)$ under an isometric operator $A$ is also dense in $\mathscr{H}$, then $A$ is unitary.*

**Proof.** Choose $f \in \mathscr{H}$ so $\exists (f_n) \subseteq \widehat{W}$ such that $f_n \to f$. Now, since $A$ is isometric, it is $1:1$, so for every $f_n$, there is a unique $g_n \in W$ such that $f_n = Ag_n$. Also since $A$ is isometric, $g_n$ must also be convergent to some $g \in \mathscr{H}$ and since $A$ is continuous, $f = Ag$. Hence $A$ is onto. ■

Thus, since $F$ is unitary on the dense subspace $S(\mathbb{R})$, $U_F$ is a unitary operator on $L^2(\mathbb{R})$. It also follows that the inverse Fourier transform can be extended to $L^2(\mathbb{R})$ and that its extension is $U_F^{-1}$. We note that for an arbitrary $L^2$ function, the integral definition of the Fourier transform may not be correct as the integral need not exist.

## 3.2 Coordinate Operators

### 3.2.1 The Position Operator

We have also already introduced the one-dimensional position operator $x$ and have claimed that it represents the observable quantity of position of a particle, and must therefore be self-adjoint. We will now justify this assertion. Recall that we defined $x$ to be the multiplication operator on $L^2(\mathbb{R})$:

$$(xf)(x) = xf(x), \quad \mathscr{D}_x = \left\{ f \in \mathscr{H} : \int_{\mathbb{R}} |xf(x)|^2 dx < \infty \right\}$$

(see section 2.1.1). We immediately derive that

$$\langle f, xg \rangle = \int_{\mathbb{R}} \overline{f(x)} xg(x)\, dx = \int_{\mathbb{R}} \overline{xf(x)} g(x)\, dx = \langle xf, g \rangle$$

so $x$ is symmetric. Thus, the Cayley transform of $x$, $V = (x-i)(x+i)^{-1}$ is isometric from $\mathscr{R}_{x+i}$ to $\mathscr{R}_{x-i}$. However, given $f \in L^2(\mathbb{R})$, the functions $g_\pm(x) = f(x)/(x \pm i)$ are square-integrable:

$$\int_{\mathbb{R}} \left| \frac{f(x)}{x \pm i} \right|^2 dx \leqslant \int_{\mathbb{R}} |f(x)|^2 dx < \infty$$

since $|x \pm i| \geqslant 1$ for $x \in \mathbb{R}$. Clearly $(x \pm i) g_\pm = f$ so $f \in \mathscr{R}_{x \pm i}$. That is, $\mathscr{R}_{x \pm i} = L^2(\mathbb{R})$ so $V$ is a unitary operator on $L^2(\mathbb{R})$. Therefore, $x$ must be self-adjoint by theorem 9.

Let us now investigate the spectrum of the position operator. The position operator has no eigenvalues since

$$\begin{aligned} xf &= \lambda f \quad \Rightarrow \quad \|(x-\lambda) f\| = 0 \quad \Rightarrow \quad \int_{\mathbb{R}} |(x-\lambda) f(x)|^2 dx = 0 \\ &\Rightarrow \quad |x-\lambda|^2 f(x) = 0 \text{ ae} \quad \Rightarrow \quad f(x) = 0 \text{ ae.} \end{aligned}$$

Hence the point spectrum $\sigma_p(x)$ is empty.

However, in an extremely loose sense, the *Dirac delta functions* $\delta(x-\lambda)$ can be thought of as 'eigenfunctions' corresponding to the real eigenvalue $\lambda$ since

$$\int_{\mathbb{R}} x\delta(x-\lambda)\, dx = \lambda = \int_{\mathbb{R}} \lambda \delta(x-\lambda)\, dx$$

in a distributional sense [25] ($\lambda$ must be real so that it falls within the range of integration). That is, $x\delta(x-\lambda) = \lambda\delta(x-\lambda)$. Following this intuitive idea then, we take for each $\lambda \in \mathbb{R}$ the sequence of $L^2$ functions $\varphi_n(x) = n\chi_{[\lambda, \lambda+1/n]}(x)$ ($\chi_A$ is the characteristic function of the set $A$) which 'approximate' the delta function $\delta(x-\lambda)$. Then,

$$\|(x-\lambda)\varphi_n\|^2 = n^2 \int_\lambda^{\lambda+1/n} (x-\lambda)^2 dx = \frac{1}{3n} \to 0 \text{ as } n \to \infty.$$

Therefore, $(x-\lambda)\varphi_n \to 0$ but $\varphi_n \nrightarrow 0$ so the inverse operator $(x-\lambda)^{-1}$ cannot be continuous and is thus unbounded. By the discussion of section 2.4 then, $\lambda \in \sigma_c(x)$.

Therefore, the spectrum of the position operator is wholly continuous and consists of the entire real axis. This corresponds to the intuitive idea that the position of a free particle in one dimension may be anywhere and that the position is not discretised as say, the energy levels of an atom are known to be.

We shall conclude our discussion of the position operator by noting that if we use the spectral theorem (theorem 17) to write

$$\langle f, xg\rangle = \int_{\mathbb{R}} \lambda \, d\langle f, E_\lambda g\rangle$$

where $E_\lambda$ is the spectral function associated with $x$, and use the functional calculus also, we can derive that

$$\langle f, E(B)g\rangle = \int_B d\langle f, E_\lambda g\rangle = \int_{\mathbb{R}} \chi_B(\lambda)\, d\langle f, E_\lambda g\rangle = \langle f, \chi_B(x) g\rangle. \tag{3.3}$$

That is, the projector-valued spectral measure associated with $x$, $E(B)$, is just multiplication by the characteristic function $\chi_B(x)$.

### 3.2.2 The Momentum Operator

Let us now define the one-dimensional momentum operator $p$ by $p = U_F^{-1} x U_F$ where $U_F$ is the Fourier operator acting on $L^2(\mathbb{R})$. That is, whereas $x$ is a multiplication operator in coordinate space, $p$ is the corresponding multiplication operator in the Fourier domain, or what is generally known in physics as momentum space. The domain of $p$ is therefore

$$\mathscr{D}_p = \left\{ f : \int_{\mathbb{R}} k^2 \left|\widehat{f}(k)\right|^2 dk < \infty \right\}.$$

This is justified by noting that given any $f \in \mathscr{D}_p$,

$$\widehat{(pf)} = U_F\left(U_F^{-1} x U_F f\right) = x\widehat{f} \quad \Rightarrow \quad \widehat{(pf)}(k) = k\widehat{f}(k).$$

The symmetry of $p$ follows immediately from that of $x$ and the unitarity of $U_F$ :

$$\langle f, pg\rangle = \left\langle f, U_F^{-1} x U_F g\right\rangle = \langle U_F f, x U_F g\rangle = \langle x U_F f, U_F g\rangle = \left\langle U_F^{-1} x U_F f, g\right\rangle = \langle pf, g\rangle,$$

and it is easy to see that $p$ is densely defined so $p^\dagger$ exists.

The representation of the momentum operator in coordinate space is also easily derived. However, since the integral form for the Fourier operator does not hold for all $L^2$ functions, we must also restrict the momentum operator to achieve a nice representation. Let $f \in S(\mathbb{R})$. Then,

$$\begin{aligned}(pf)(x) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} k\widehat{f}(k) e^{ikx} dk = \frac{-i}{\sqrt{2\pi}} \int_{\mathbb{R}} \frac{\partial}{\partial x}\left(\widehat{f}(k) e^{ikx}\right) dk \\ &= -i\frac{\partial}{\partial x}\left[\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \widehat{f}(k) e^{ikx} dk\right] = -i\frac{\partial}{\partial x} f(x)\end{aligned} \tag{3.4}$$

where the interchange of integration and differentiation is justified by Leibniz's rule and the properties of $S(\mathbb{R})$ [36].

We can now easily show that $p$ is an unbounded operator. Let us define $\varphi_n(x) = \sqrt{n} e^{-\pi n^2 x^2/2}$ for each positive integer $n$. Then, $\|\varphi_n\| = 1$ for every $n$ and $\varphi_n \in S(\mathbb{R})$. However,

$$\|p\varphi_n\|^2 = \left\|\varphi_n'\right\|^2 = \int_{\mathbb{R}} \left|\varphi_n'(x)\right|^2 dx = \pi^2 n^5 \int_{\mathbb{R}} x^2 e^{-\pi n^2 x^2} dx = \frac{\pi n^2}{2}.$$

Thus $\|p\varphi_n\| \to \infty$ as $n \to \infty$ and so $p$ is unbounded.

We have already shown that $p \subseteq p^\dagger$. To see the converse, we use the relations [27]

$$(AB)^\dagger \supseteq B^\dagger A^\dagger \qquad ; \qquad A \subseteq B \quad \Rightarrow \quad UA \subseteq UB, AU \subseteq BU$$

where $A$, $B$ and $AB$, are densely defined and $U$ is unitary. Now, $x = U_F p U_F^{-1}$ so $x^\dagger = x = \left(U_F p U_F^{-1}\right)^\dagger \supseteq U_F p^\dagger U_F^{-1}$. Since the Fourier operator and its inverse are unitary, we have $U_F^{-1} x U_F \supseteq p^\dagger$ which is just $p \supseteq p^\dagger$. Thus $p$ is self-adjoint.

To summarise then, we have now also shown that both $x$ and $p$ are unbounded self-adjoint operators in $L^2(\mathbb{R})$. With regards to the spectrum of $p$, we recall from section 2.4 that $\lambda \notin \sigma(p)$ iff $p - \lambda$ has a bounded inverse. This is clearly equivalent to requiring that $U_F(p-\lambda)U_F^{-1}$ has a bounded inverse which will be the case iff $U_F p U_F^{-1} - \lambda = x - \lambda$ has a bounded inverse. Thus $\sigma(p) = \sigma(x) = \mathbb{R}$, the real line. In fact, the point spectrum is empty by a similar argument where the word bounded is removed, so the spectrum of $p$ is wholly continuous also. As in the case of the position operator, we associate this result with the intuitive idea that momenta are not discretised. Furthermore, if $E_\lambda^x$ and $E_\lambda^p$ are the spectral functions of $x$ and $p$ respectively, then we also have the relation:

$$\langle f, pg \rangle = \langle U_F f, x U_F g \rangle = \int_{\mathbb{R}} \lambda \, d\langle U_F f, E_\lambda^x U_F g \rangle = \int_{\mathbb{R}} \lambda \, d\langle f, U_F^{-1} E_\lambda^x U_F g \rangle$$

so $E_\lambda^p = U_F^{-1} E_\lambda^x U_F$.

## 3.3 Energy Operators

### 3.3.1 The Kinetic Energy Operator

The kinetic energy of a non-relativistic particle of mass $m$ is classically related to the momentum $p$ of the particle by $K = p^2/2m$. If we use units in which the mass of the particle is $1/2$ (just as we choose units in which $\hbar = 1$) then this is just $K = p^2$. Analogously, the kinetic energy of a quantum system (with $m = 1/2$) is represented by the operator $H_0 = p^2$, called the *free Hamiltonian* of the system. Since $H_0$ is a real-valued (unbounded) function of the self-adjoint operator $p$, $H_0$ is also self-adjoint (and unbounded) by theorem 19. (that $H_0$ is densely defined is clear and shown below). We also note that in momentum space, $H_0$ is just multiplication by $k^2$ :

$$\widehat{H_0 f}(k) = \widehat{ppf}(k) = k\widehat{pf}(k) = k^2 \widehat{f}(k).$$

The spectrum of $H_0$ must lie on the real axis and it is easy to see that $H_0 = p^2 = U_F^{-1} x^2 U_F$. Therefore by the discussion of the previous section, the spectra of $H_0$ and $x^2$ are identical. It is also easy to check that $x^2$ has no eigenvalues, so $\sigma_p(H_0)$ is empty.

Suppose that $\lambda < 0$. If we choose any $\varphi \in L^2(\mathbb{R})$, then

$$\left\| \left(x^2 - \lambda\right) \varphi \right\|^2 = \int_{\mathbb{R}} \left(x^2 - \lambda\right)^2 |\varphi(x)|^2 \, dx \geqslant \lambda^2 \int_{\mathbb{R}} |\varphi(x)|^2 \, dx = \lambda^2 \|\varphi\|^2$$

since $\left(x^2 - \lambda\right) \geqslant |\lambda|$. Therefore $x^2 - \lambda$ is bounded below so $\left(x^2 - \lambda\right)^{-1}$ is bounded above. That is, $x^2 - \lambda$ has a bounded inverse and $\lambda \notin \sigma(H_0)$.

However, if $\lambda \geqslant 0$, we can take the sequence $\varphi_n(x) = \sqrt{n}\chi_{\left[\sqrt{\lambda}, \sqrt{\lambda}+1/n\right]}(x)$, so that $\|\varphi_n\| = 1$ for all $n$ but

$$\left\| \left(x^2 - \lambda\right) \varphi_n \right\|^2 = n \int_{\sqrt{\lambda}}^{\sqrt{\lambda}+1/n} \left(x^2 - \lambda\right)^2 dx = \frac{20\lambda n^2 + 15\sqrt{\lambda} n + 3}{15 n^4} \to 0 \text{ as } n \to \infty$$

so $\left(x^2 - \lambda\right) \varphi_n \to 0$ but $\varphi_n \nrightarrow 0$. Therefore $\left(x^2 - \lambda\right)^{-1}$ is not continuous and so $\lambda \in \sigma_c(H_0)$.

We have thus shown that the spectrum of the free Hamiltonian is purely continuous and runs from 0 to $\infty$. Physically, this allows the free (unbound) particle to take any positive energy, which is exactly what one expects.

Now, recall that in coordinate space, $p$ has the differential form $-i\partial/\partial x$ on the functions of rapid decrease $S(\mathbb{R})$. However, we have no guarantee that this restriction of $p$ is self-adjoint. But, we can conclude that $H_0 = p^2$ has the form $-\partial^2/\partial x^2$ on $S(\mathbb{R})$ and in fact, this is the representation which is usually first encountered in elementary quantum theory. This restricted operator is also not self-adjoint (although it is easy to check that it is symmetric). What we now show is that $H_0$ is actually an extension of the operator $T = -\partial^2/\partial x^2$ defined on $S(\mathbb{R})$, just as $p$ is an extension of the operator $-i\partial/\partial x$ defined on $S(\mathbb{R})$.

Let $f \in S(\mathbb{R}) = \mathscr{D}_T$ be of rapid decrease. Then, $\widehat{H_0 f}(k) = k^2 \widehat{f}(k)$ is also of rapid decrease so $f \in \mathscr{D}_{H_0}$. Thus $H_0$ is densely defined so self-adjoint as claimed above. Furthermore, using the properties of $S(\mathbb{R})$, we have

$$\begin{aligned}(Tf)(x) &= \frac{-1}{\sqrt{2\pi}}\frac{\partial^2}{\partial x^2}\int_{\mathbb{R}} \widehat{f}(k)\, e^{ikx} dx = \frac{-i}{\sqrt{2\pi}}\frac{\partial}{\partial x}\int_{\mathbb{R}} k\widehat{f}(k)\, e^{ikx} dx \\ &= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} k^2 \widehat{f}(k)\, e^{ikx} dx = (H_0 f)(x)\end{aligned}$$

so $T \subseteq H_0$.

Furthermore, we can also show that $H_0$ is the closure of $T$.

**Lemma 21** *The set $(I+T)S(\mathbb{R}) = \{f : f = g + Tg \text{ for some } g \in S(\mathbb{R})\}$ is dense in $L^2(\mathbb{R})$.*

**Proof.** Suppose $h$ is orthogonal to $(I+T)S(\mathbb{R})$ so

$$\int_{\mathbb{R}} \widehat{h}(k)\left(1+k^2\right)\widehat{g}(k)\, dk = 0$$

for any $\widehat{g} \in S(\mathbb{R})$. Then, $\widehat{h}(k)\left(1+k^2\right)$ must be orthogonal to $S(\mathbb{R})$, so by denseness, $\widehat{h}(k)\left(1+k^2\right) = 0$ ae, so $\widehat{h}(k) = 0$ ae, so $h = 0$. Therefore, $(I+T)S(\mathbb{R})$ must also be dense in $L^2(\mathbb{R})$. ■

**Theorem 22** *$H_0$ is the closure of the differential operator $T = -\dfrac{\partial^2}{\partial x^2}$ defined on $S(\mathbb{R})$.*

**Proof.** Let $f \in \mathscr{D}_{H_0}$. Then, since $(I+T)S(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, we can find a $g_n \in S(\mathbb{R})$ such that $\|(I+H_0)f - (I+T)g_n\| < 1/n$. Since $Tg_n = H_0 g_n$, this is equivalent to $\|(I+H_0)(f-g_n)\| < 1/n$. Now, because $\left(1+k^2\right) \geqslant 1$,

$$\begin{aligned}\|f-g_n\|^2 = \int_{\mathbb{R}} \left|\widehat{f}(k) - \widehat{g_n}(k)\right|^2 dk &\leqslant \int_{\mathbb{R}} \left(1+k^2\right)^2 \left|\widehat{f}(k) - \widehat{g_n}(k)\right|^2 dk \\ &= \|(I+H_0)(f-g_n)\|^2 < \frac{1}{n^2}.\end{aligned}$$

We also have

$$\begin{aligned}\|H_0 f - Tg_n\|^2 = \|H_0(f-g_n)\|^2 &= \int_{\mathbb{R}} k^4 \left|\widehat{f}(k) - \widehat{g_n}(k)\right|^2 dk \\ \leqslant \int_{\mathbb{R}} \left(1+k^2\right)^2 \left|\widehat{f}(k) - \widehat{g_n}(k)\right|^2 dk &= \|(I+H_0)(f-g_n)\|^2 < \frac{1}{n^2}.\end{aligned}$$

Therefore, $g_n \to f$ and $Tg_n \to H_0 f$. But, $T$ is symmetric and thus has a closure $\overline{T}$. By definition then, $f \in \mathscr{D}_{\overline{T}}$ and $Tg_n = \overline{T}g_n \to \overline{T}f$. By uniqueness of limits then, $\overline{T}f = H_0 f$ for all $f \in \mathscr{D}_{H_0}$ so $H_0 \subseteq \overline{T}$. Finally however, $H_0$ is a self-adjoint, hence closed, extension of $T$ so $H_0 \supseteq \overline{T}$ by definition. That is, $H_0 = \overline{T}$. ■

It will be more convenient to work in three dimensions from here on with $\mathbf{r} = (x,y,z)$, and $\mathbf{k} = (k_x, k_y, k_z)$. This is because the results obtained in the following section are now *not* entirely independent of the dimension of the underlying field ($\mathbb{R}^n$) and three dimensions are what we really want to study. With this assumption, we need three position operators, $x$, $y$ and $z$, and three momentum operators $p_x$, $p_y$ and $p_z$ corresponding to the three orthogonal spatial directions. The kinetic energy operator is therefore defined to be $H_0 = p_x^2 + p_y^2 + p_z^2$ and is an extension of the negative Laplacian operator:

$$H_0 \supseteq -\nabla^2 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}. \tag{3.5}$$

### 3.3.2 The Potential Energy Operator

The potential energy between two particles usually depends upon the relative distance between them. Consequently, we shall consider potential energy operators of the form $V = V(r)$. That is, functions of the position operator $r = |\mathbf{r}| = \left(x^2 + y^2 + z^2\right)^{1/2}$. The functional calculus then ensures that $V$ is self-adjoint when $V(r)$ is real. However, the real interest lies with the total energy - the sum of the kinetic and potential energies. The problem is that we cannot use the functional calculus to conclude that $H_0 + V$ is self-adjoint on $\mathscr{D}_{H_0} \cap \mathscr{D}_V$ because $H_0$ is a function of $p_x$, $p_y$ and $p_z$ whereas $V$ is a function of $x$, $y$ and $z$, but $p_x$ and $x$ are incompatible operators (section 2.3.1) (as are $p_y$ and $y$, and $p_z$ and $z$). One way around this problem is to treat $V$ as a *perturbation* of the self-adjoint operator $H_0$. A reasonably simple method of arriving at the desired conclusion utilises the concept of *relative bounds* which we shall discuss below. We will use this to show that $H_0 + V$ is self-adjoint in the next section. Other more sophisticated methods and more general perturbations are discussed at length in [2], [26] and [40].

Consider an operator $A$. The operator $K$ is *bounded relative to* $A$ or *$A$-bounded* if $\mathscr{D}_A \subseteq \mathscr{D}_K$ and there exists $a, b \geqslant 0$ such that $\|Kf\| \leqslant a\|Af\| + b\|f\|$ for every $f \in \mathscr{D}_A$. The infimum of all $a$ such that there is a $b$ satisfying this inequality is called the *$A$-bound* of $K$. We can easily see that in the case where $K$ is bounded, $\mathscr{D}_A \subseteq \mathscr{D}_K$ (which is the whole Hilbert space) and $\|Kf\| \leqslant 0\|Af\| + \|K\|\|f\|$. Hence $K$ is $A$-bounded with $A$-bound 0. Not all potential energy operators are bounded however (eg the Coulomb potential which has the form $V(r) \sim r^{-1}$).

**Lemma 23** *For every $a > 0$, there is a $b > 0$ such that $\|f\|_\infty \leqslant a\|H_0 f\| + b\|f\|$ for every $f \in S\left(\mathbb{R}^3\right)$, where $\|f\|_\infty = \inf\{C : |f(\mathbf{r})| \leqslant C \text{ ae}\}$.*

**Proof.** Let $g(\mathbf{k}) = 1 + k^2 = 1 + k_x^2 + k_y^2 + k_z^2$, $f \in S\left(\mathbb{R}^3\right)$ and $\widehat{h}(k) = n^3 \widehat{f}(nk)$ where $n > 0$ is arbitrary. Recalling that $\|\cdot\|_1$ is the $L^1$-norm (section 1.2.2), we have that

$$\left\|\widehat{h}\right\|_1 = \left\|\widehat{f}\right\|_1, \qquad \left\|\widehat{h}\right\| = n^{3/2}\left\|\widehat{f}\right\|, \qquad \left\|k^2\widehat{h}\right\| = n^{-1/2}\left\|\widehat{f}\right\|$$

$$\text{and} \quad \left\|\widehat{h}\right\|_1 = \left\|g^{-1}\left(g\widehat{h}\right)\right\|_1 \leqslant \left\|g^{-1}\right\|\left\|g\widehat{h}\right\| \leqslant \left\|g^{-1}\right\|\left[\left\|\widehat{h}\right\| + \left\|k^2\widehat{h}\right\|\right].$$

Therefore, since $\left\|g^{-1}\right\| = \pi$,

$$\left\|\widehat{f}\right\|_1 = \left\|\widehat{h_n}\right\|_1 \leqslant \pi\left[\left\|\widehat{h_n}\right\| + \left\|k^2\widehat{h_n}\right\|\right] = \pi\left[n^{3/2}\left\|\widehat{f}\right\| + n^{-1/2}\left\|k^2\widehat{f}\right\|\right].$$

Using the isometry of the Fourier transform operator and the relation

$$|f(\mathbf{r})| \leqslant \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\left|\widehat{f}(\mathbf{k})\,e^{i\mathbf{k}\cdot\mathbf{r}}\right|d\mathbf{k} = \frac{1}{(2\pi)^{3/2}}\left\|\widehat{f}\right\|_1 \quad \Rightarrow \quad \|f\|_\infty \leqslant \frac{1}{(2\pi)^{3/2}}\left\|\widehat{f}\right\|_1,$$

we finally get

$$\|f\|_\infty \leqslant \frac{1}{\sqrt{8\pi}}\left[n^{-1/2}\|H_0 f\| + n^{3/2}\|f\|\right].$$

Thus for any $a = 1/\sqrt{8n\pi} > 0$, there is a $b = n^{3/2}/\sqrt{8\pi} = 1/\left(64\pi^2 a^3\right) > 0$ satisfying the statement of the lemma. ■

**Theorem 24 (Kato)** *Suppose that $V = V(\mathbf{r})$ has the form $V_1(\mathbf{r}) + V_2(\mathbf{r})$ where $V_1(\mathbf{r})$ is a square-integrable function and $V_2(\mathbf{r})$ is a bounded function. Then, $V$ has $H_0$-bound of 0.*

**Proof.** If $f \in S\left(\mathbb{R}^3\right)$ then

$$\|Vf\| \leqslant \|V_1 f\| + \|V_2 f\| \leqslant \|V_1(\mathbf{r})\|\,\|f\|_\infty + \|V_2(\mathbf{r})\|_\infty\|f\| \tag{3.6}$$

where $\|V_1(\mathbf{r})\|$ and $\|V_2(\mathbf{r})\|_\infty$ refer to the appropriate norms of the functions $V_1(\mathbf{r})$ and $V_2(\mathbf{r})$. By lemma 23 however, for every $a > 0$ there is a $b > 0$ such that $\|f\|_\infty \leqslant a\|H_0 f\| + b\|f\|$. Substitution into 3.6 then gives

$$\begin{aligned}\|Vf\| &\leqslant \|V_1(\mathbf{r})\|\left[a\|H_0 f\| + b\|f\|\right] + \|V_2(\mathbf{r})\|_\infty\|f\| \\ &= \left\{a\|V_1(\mathbf{r})\|\right\}\|H_0 f\| + \left\{b + \|V_2(\mathbf{r})\|_\infty\right\}\|f\|.\end{aligned}$$

Thus $\|Vf\|$ is finite (and so $f \in \mathscr{D}_V$), and $V$ has $H_0$-bound 0 on $S\left(\mathbb{R}^3\right)$.
We now extend this result from $S\left(\mathbb{R}^3\right)$ to $\mathscr{D}_{H_0}$. Let $g \in \mathscr{D}_{H_0}$. By a similar argument to lemma 21, the set $H_0\left[S\left(\mathbb{R}^3\right)\right]$ is also dense in $L^2\left(\mathbb{R}^3\right)$ so we can take a sequence $(g_n) \subseteq S\left(\mathbb{R}^3\right)$ such that $g_n \to g$ and (using the fact that $H_0$ is closed) $H_0 g_n \to H_0 g$. Now, for every $\alpha > 0$ there is a $\beta > 0$ such that

$$\|V(g_n - g_m)\| \leqslant \alpha \|H_0(g_n - g_m)\| + \beta \|(g_n - g_m)\|$$

so $Vg_n$ is also convergent. But, $V$ is self-adjoint hence closed. Hence $g \in \mathscr{D}_V$ and $Vg_n \to Vg$. Therefore, $\mathscr{D}_{H_0} \subseteq \mathscr{D}_V$. Finally, we also have

$$\|Vg\| \leqslant \|Vg_n\| + \|V(g - g_n)\| \leqslant \alpha \|H_0 g_n\| + \beta \|g_n\| + \|V(g - g_n)\|$$

so as $n \to \infty$, we get that for an arbitrary $g \in \mathscr{D}_{H_0}$ and every $\alpha > 0$ there is a $\beta > 0$ such that

$$\|Vg\| \leqslant \alpha \|H_0 g\| + \beta \|g\|.$$

■

There is also an extension of this theorem [26] which establishes a similar result when $V$ is the sum of $n$ potentials of the type discussed above. Then, $V$ has $H_0$-bound 0 on $S\left(\mathbb{R}^{3n}\right)$.

### 3.3.3 The Hamiltonian Operator

We are now in a position to define rigorously the total energy or *Hamiltonian* operator of a quantum system. This is the operator $H = H_0 + V$, and is of course generally unbounded. To prove that it is self-adjoint so that we may legitimately associate the observable quantity of energy with it, we need the following lemma [20].

**Lemma 25 (Spectral Radius)** *For any bounded operator $A$,*

$$\sigma(A) \subseteq \{\lambda \in \mathbb{C} : |\lambda| \leqslant \|A\|\}.$$

**Theorem 26 (Kato-Rellich)** *Suppose $V$ has $H_0$-bound 0. Then, $H = H_0 + V$ is self-adjoint on $\mathscr{D}_H = \mathscr{D}_{H_0}$.*

**Proof.** Let us choose a real $\lambda \neq 0$. Then, since $H_0$ is self-adjoint, $\pm\lambda i \notin \sigma(H_0)$ so $(H_0 \pm \lambda i)^{-1}$ exists and is defined everywhere ($\mathscr{R}_{H_0 \pm \lambda i} = L^2\left(\mathbb{R}^3\right)$). It is clear that $(H_0 \pm \lambda i)^{-1} f \in \mathscr{D}_{H_0} \subseteq \mathscr{D}_V$ for any $f \in L^2\left(\mathbb{R}^3\right)$, so for arbitrarily small $a > 0$, there is a $b > 0$ such that

$$\left\|V(H_0 \pm \lambda i)^{-1} f\right\| \leqslant a \left\|H_0(H_0 \pm \lambda i)^{-1} f\right\| + b \left\|(H_0 \pm \lambda i)^{-1} f\right\| \tag{3.7}$$

since $V$ has $H_0$-bound 0. Using equation 2.1, we derive that

$$\|f\|^2 = \left\|H_0(H_0 \pm \lambda i)^{-1} f\right\|^2 + \lambda^2 \left\|(H_0 \pm \lambda i)^{-1} f\right\|^2$$

and hence that

$$\|f\| \geqslant \left\|H_0(H_0 \pm \lambda i)^{-1} f\right\| \text{ and } \|f\| \geqslant |\lambda| \left\|(H_0 \pm \lambda i)^{-1} f\right\|$$

for any $f \in L^2\left(\mathbb{R}^3\right)$. Substituting into equation 3.7, we have

$$\left\|V(H_0 \pm \lambda i)^{-1} f\right\| \leqslant \left(a + \frac{b}{|\lambda|}\right) \|f\|.$$

By choosing $a < 1$, we obtain $\left\|V(H_0 \pm \lambda i)^{-1} f\right\| < \|f\|$ for $|\lambda|$ sufficiently large. It follows that for such a $\lambda$, $\left\|V(H_0 \pm \lambda i)^{-1}\right\| < 1$ so by lemma 25, $-1 \notin \sigma\left(V(H_0 \pm \lambda i)^{-1}\right)$. Hence

$V(H_0 \pm \lambda i)^{-1} + 1$ has a bounded inverse so $\mathscr{R}_{V(H_0\pm\lambda i)^{-1}+1} = L^2(\mathbb{R}^3) = \mathscr{R}_{H_0\pm\lambda i}$. It follows then that

$$\mathscr{R}_{\left(V(H_0\pm\lambda i)^{-1}+1\right)(H_0\pm\lambda i)} = \mathscr{R}_{V+H_0\pm\lambda i} = L^2(\mathbb{R}^3).$$

Now we know that $\lambda^{-1}(H_0+V)$ is symmetric on $\mathscr{D}_{H_0}$ so its Cayley transform,

$$U = \left[\lambda^{-1}(H_0+V) - i\right]\left[\lambda^{-1}(H_0+V) + i\right]^{-1} = (V+H_0-\lambda i)(V+H_0+\lambda i)^{-1}$$

is isometric. But, we have just shown that $U$ is actually unitary for $|\lambda|$ sufficiently large ($\mathscr{R}_{V+H_0\pm\lambda i} = L^2(\mathbb{R}^3)$) so $\lambda^{-1}(H_0+V)$, and therefore $H = H_0+V$, must be self-adjoint on $\mathscr{D}_H = \mathscr{D}_{H_0}$. ■

To illustrate this result, we shall take the Coulomb potential in three-dimensions which takes the form (ignoring a few constants), $V(r) = r^{-1}$. This potential may be written

$$V(r) = \frac{\chi(r)}{r} + \frac{1-\chi(r)}{r}$$

where $\chi(r)$ is the characteristic function of the set $\{\mathbf{r} : r < 1\}$. Clearly, the second term is bounded by 1 whereas the first term is square-integrable:

$$\int_{\mathbb{R}^3} \frac{\chi(r)}{r} d\mathbf{r} = \int_0^{2\pi}\int_0^{\pi}\int_0^1 \frac{1}{r} r^2 \sin\theta \, dr d\theta d\phi = 4\pi \int_0^1 r dr < \infty.$$

Therefore by theorems 24 and 26, $H = H_0 + V$ is a self-adjoint operator on $\mathscr{D}_{H_0}$.

The concept of relative bounds is also very useful in studying other properties of the Hamiltonian operator. As an example, this can be used to prove that the spectrum of $H$ is bounded below (as $H_0$ is), showing that the theory demands the concept of a ground state energy. This and other properties including the problem important in scattering theory of when the continuous spectrum of $H$ is the whole positive real axis (as it is for $H_0$) are treated in [40] and [26].

For a typical potential that we will be studying, the spectrum of $H$ is continuous from 0 to $\infty$ and the point spectrum consists of negative eigenvalues which may have only 0 as a limit point. We associate the bound states of the potential with the point spectrum (the energies of the bound states being the eigenvalues) and we associate the unbound states with the continuous spectrum. It is these unbound states which are important in scattering theory.

# Chapter 4

# Two-Body Scattering Theory

*"Rigorous proofs of dispersion relations are like breasts on a man, neither useful nor ornamental."*
M L Goldberger

## 4.1 Revisiting the Schrödinger Equation

Recall the discussion of section 1.1.2. There we briefly discussed solving scattering problems using the Schrödinger equation 1.1 (with $\hbar = 1$)

$$i\frac{\partial \Psi}{\partial t} = H\Psi$$

and also mentioned why this is generally not entirely satisfactory. We can now also see that because $H$ is unbounded and thus not defined on the whole Hilbert space, this equation cannot be correct for all possible $\Psi$. In fact, this equation is essentially postulating that the operator $H$ acts on some domain like the differential operator $i\partial/\partial t$. However, it is possible to reformulate this *dynamical law of motion* so that it is applicable to all $\Psi$. This therefore must be done with the aid of a *bounded* operator.

### 4.1.1 The Time-Evolution Operator

If we were to formally solve the Schrödinger equation (pretending $H$ is just a constant - we shall assume throughout that $H$ does not depend on time explicitly), we would arrive at the solution $\Psi(t) = e^{-iHt}\Psi(0)$. We shall therefore refer to $e^{-iHt}$ as a *time-evolution operator*. Because $e^{-i\lambda t}\overline{e^{-i\lambda t}} = 1$, we have $e^{-iHt}\left(e^{-iHt}\right)^\dagger = \left(e^{-iHt}\right)^\dagger e^{-iHt} = I$ by the functional calculus. Thus $e^{-iHt}$ is unitary hence bounded for each $t$. Furthermore, if $H$ has spectral function $E_\lambda$ then we have

$$\left\langle f, e^{-iHt}g\right\rangle = \int_{\mathbb{R}} e^{-i\lambda t}d\left\langle f, E_\lambda g\right\rangle \qquad (f,g \in \mathscr{D}_H)$$

from which it follows that $e^{-iHt} = I$ when $t = 0$ and $e^{-iHt_1}e^{-iHt_2} = e^{-iH(t_1+t_2)}$ by a simple application of the extension principle for bounded operators. Reflection will show that this additivity is what we expect of a time-evolution operator. We will now show that $\Psi(t) = e^{-iHt}\Psi(0)$ is a generalisation of the Schrödinger equation by showing that $\Psi(t)$ satisfies equation 1.1 whenever $\Psi(0) \in \mathscr{D}_H$.

Suppose that $\Psi(0) \in \mathscr{D}_H$. We know that $e^{-iHt}$ is unitary and commutes with $E_\lambda$ so

$$\left\|H\left[e^{-iHt}\Psi(0)\right]\right\|^2 = \int_{\mathbb{R}} \lambda^2 d\left\|E_\lambda\left[e^{-iHt}\Psi(0)\right]\right\|^2 = \int_{\mathbb{R}} \lambda^2 d\left\|E_\lambda\Psi(0)\right\|^2 = \left\|H\Psi(0)\right\|^2 < \infty$$

and thus $\Psi(t) = e^{-iHt}\Psi(0) \in \mathscr{D}_H$. Therefore, we can write

$$i\frac{\partial}{\partial t}\left[e^{-iHt}\Psi(0)\right] = i\lim_{h\to 0}\frac{e^{-iH(t+h)} - e^{-iHt}}{h}\Psi(0) = i\lim_{h\to 0}\frac{e^{-iHh} - I}{h}e^{-iHt}\Psi(0). \tag{4.1}$$

Now, the identity $\lim_{h\to 0} h^{-1}\left(e^{-i\lambda h}-1\right)=-i\lambda$ is easily established and we also have

$$\left\|\left(\frac{e^{-iHh}-I}{h}+iH\right)f\right\|^2=\int_{\mathbb{R}}\left|\frac{e^{-i\lambda h}-1}{h}+i\lambda\right|^2 d\left\|E_\lambda f\right\|^2$$

for any $f\in\mathscr{D}_H$. Since

$$\left|\frac{e^{-i\lambda h}-1}{h}+i\lambda\right|^2=\left|e^{-i\lambda h/2}\frac{-i\sin(\lambda h/2)}{h/2}+i\lambda\right|^2\leqslant\left[\left|\frac{\sin(\lambda h/2)}{h/2}\right|+|\lambda|\right]^2\leqslant 4\lambda^2$$

is integrable with respect to the measure $\|E_\lambda f\|^2$ (because $f\in\mathscr{D}_H$), we get

$$\lim_{h\to 0}\left\|\left(\frac{e^{-iHh}-I}{h}+iH\right)f\right\|^2=0$$

using dominated convergence. Therefore, $h^{-1}\left(e^{-iHh}-I\right)\to -iH$ strongly as $h\to 0$, and substituting back into 4.1 gives

$$i\frac{\partial}{\partial t}\left[e^{-iHt}\Psi(0)\right]=i\lim_{h\to 0}\frac{e^{-iHh}-I}{h}e^{-iHt}\Psi(0)=H\left[e^{-iHt}\Psi(0)\right].$$

As claimed then, $\Psi(t)=e^{-iHt}\Psi(0)$ satisfies the Schrödinger equation whenever $\Psi(0)\in\mathscr{D}_H$.

### 4.1.2 The Green's Operators

Consider now the eigenvalue problem for the energy of the system. This requires us to solve the *time independent Schrödinger equation*

$$H\Psi=(H_0+V)\Psi=E\Psi\quad\Rightarrow\quad(E-H_0)\Psi=V\Psi$$

where $E$ is the energy eigenvalue. In scattering, we generally know the energy of the system but not the state $\Psi$. However, from this we might conclude that a knowledge of the inverse operator $(E-H_0)^{-1}$ may be useful for studying $\Psi$. To this end then, we introduce the *free Green's operator*,

$$G_0(E)=(E-H_0)^{-1}.$$

We note immediately that the free Green's operator does not exist (section 2.4) when $E\in\sigma_p(H_0)$, and is unbounded (hence not everywhere defined) when $E\in\sigma_c(H_0)$. Therefore, we shall only define $G_0(E)$ for $\mathrm{Im}E\neq 0$, ensuring boundedness.

Now, $G_0(E)$ operates in momentum space as a multiplication operator:

$$\left(G_0(E)\Psi\right)\hat{}\,(\mathbf{k})=\left((E-H_0)^{-1}\Psi\right)\hat{}\,(\mathbf{k})=\left(E-k^2\right)^{-1}\widehat{\Psi}(\mathbf{k}).$$

where we make that simplifying assumption that $m=1/2$. We can therefore Fourier transform $\left(E-k^2\right)^{-1}\widehat{\Psi}(\mathbf{k})$ to determine the action of $G_0(E)$ in coordinate space. If $\widehat{\Psi}(\mathbf{k})\in S\left(\mathbb{R}^3\right)$ then so is $\left(E-k^2\right)^{-1}\widehat{\Psi}(\mathbf{k})$ since $\left(E-k^2\right)^{-1}$ is bounded for $\mathrm{Im}E\neq 0$. Therefore, the integral representation of the inverse Fourier transform is applicable (equation 3.2). The transform is achieved using contour integration giving the result [8], [43]:

$$\left(G_0(E)\Psi\right)(\mathbf{r})=\int_{\mathbb{R}^3}G_0\left(\mathbf{r},\mathbf{r}';E\right)\Psi\left(\mathbf{r}'\right)d\mathbf{r}'\tag{4.2}$$

where $G_0(\mathbf{r},\mathbf{r}';E)=\dfrac{-1}{4\pi}\dfrac{e^{i\sqrt{E}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$ and $\mathrm{Im}\sqrt{E}>0$.

Thus $G_0(E)$ becomes an *integral operator* on $S(\mathbb{R}^3)$. The *kernel* of the operator, $G_0(\mathbf{r},\mathbf{r}';E)$, is called the free Green's function. A quick calculation shows that $G_0(\mathbf{r},\mathbf{r}';E)$ is square integrable in either (but not both) $\mathbf{r}$ or $\mathbf{r}'$ :

$$\begin{aligned}\int_{\mathbb{R}^3}\left|G_0(\mathbf{r},\mathbf{r}';E)\right|^2 d\mathbf{r} &= \frac{1}{16\pi^2}\int_{\mathbb{R}^3}\frac{e^{-2\mathrm{Im}\sqrt{E}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|^2}d\mathbf{r}\\ &= \frac{1}{16\pi^2}\int_{\mathbb{R}^3}\frac{e^{-2\mathrm{Im}\sqrt{E}|\mathbf{u}|}}{|\mathbf{u}|^2}d\mathbf{u}\\ &= \frac{1}{4\pi}\int_0^\infty\frac{e^{-2\mathrm{Im}\sqrt{E}u}}{u^2}u^2du=\frac{1}{8\pi\mathrm{Im}\sqrt{E}}.\end{aligned} \tag{4.3}$$

We shall also introduce the *full Green's operator* $G(E)=(E-H)^{-1}$. This is also an integral operator in the coordinate representation:

$$(G(E)\Psi)(\mathbf{r})=\int_{\mathbb{R}^3}G(\mathbf{r},\mathbf{r}';E)\Psi(\mathbf{r}')\,d\mathbf{r}'$$

with a kernel $G(\mathbf{r},\mathbf{r}';E)$ called the *full Green's function*, although we shall not prove this until the next chapter. The full and free Green's operators are however related by the second resolvent identity which has the form [3]

$$G(E)=G_0(E)+G_0(E)VG(E). \tag{4.4}$$

## 4.2 Time Dependent Scattering Theory

### 4.2.1 The Asymptotic Condition

We are now in a position to formulate the two-body scattering problem. It is well known that we can work in the centre of mass system where the two particle system can be described by the relative motion vector $\mathbf{r}$. For convenience we will set the *reduced mass* $m=m_1m_2/(m_1+m_2)$ to be $1/2$. On a Hilbert space level, the two-particle system should be described by the *tensor product* (see [4] or [29] for a discussion of tensor products) of $L^2(\mathbb{R}^3)$ and $L^2(\mathbb{R}^3)$, denoted by $L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)$. Factoring out the centre of mass leaves the space $L^2(\mathbb{R}^3)$.

In the time-dependent model, we visualise a system which in the distant past and future is free of any potentials (the particles are well separated hence non-interacting). We therefore postulate that the real state of the system $\Psi(t)$, must asymptotically approach free states, $\Psi_{in}(t)$ and $\Psi_{out}(t)$. That is,

$$\Psi(t)\to\Psi_{in}(t)\ \text{as}\ t\to-\infty\quad\text{and}\quad\Psi(t)\to\Psi_{out}(t)\ \text{as}\ t\to+\infty.$$

This is referred to as the *asymptotic condition*. That these asymptotic states are free suggests that a time-evolution of such states be defined by

$$\Psi_{as}(t)=e^{-iH_0t}\Psi_{as}(0).$$

where *as* refers to *in* or *out*. The real state is of course not free so it evolves under the full Hamiltonian. With these assumptions, the asymptotic condition becomes

$$\|\Psi(t)-\Psi_{as}(t)\|=\left\|e^{-iHt}\Psi(0)-e^{-iH_0t}\Psi_{as}(0)\right\|=\left\|\Psi(0)-e^{iHt}e^{-iH_0t}\Psi_{as}(0)\right\|\to 0. \tag{4.5}$$

The quantum states which are relevant to scattering are then just those states $\Psi=\Psi(0)$ for which the asymptotic condition holds. Physically, we are trying to identify states of the system for which the interaction between the particles is negligible in the distant past and future. This requires the potential energy to decrease quickly as the particles separate. The key here is decrease quickly - it turns out that for many potentials (including unfortunately the important

Coulomb potential), the decrease is not fast enough and a modified asymptotic condition must be introduced [3]. We shall discuss this briefly in section 4.5.

Nevertheless, assuming we have a quickly decreasing potential, we can define the scattering states by introducing the sets

$$\begin{aligned} M_{\pm} &= \left\{ \Psi : \lim_{t \to \mp\infty} e^{iHt} e^{-iH_0 t} \Psi \text{ exists} \right\} \\ R_{\pm} &= \left\{ \Psi_{\pm} = \lim_{t \to \mp\infty} e^{iHt} e^{-iH_0 t} \Psi : \Psi \in M_{\pm} \right\}. \end{aligned}$$

The reason for labelling $M_+$ as the limit as $t \to -\infty$ and vice-versa is partly historical (and rather annoying) and will become clearer later. It is easily checked that $R_+ \cap R_-$ represent all the actual states of the system which approach free states in the past *and* in the future (the scattering states), and that $M_{\pm}$ represent all the possible asymptotic states.

### 4.2.2 The Scattering Operators

In scattering theory, we generally know the incoming asymptotic wavefunction $\Psi_{in}(t)$ and what we measure is related to the outgoing asymptotic wavefunction $\Psi_{out}(t)$. Therefore, we are now going to define the *Møller wave operators* which map the asymptotic states to the actual ones (see figure 4.1).

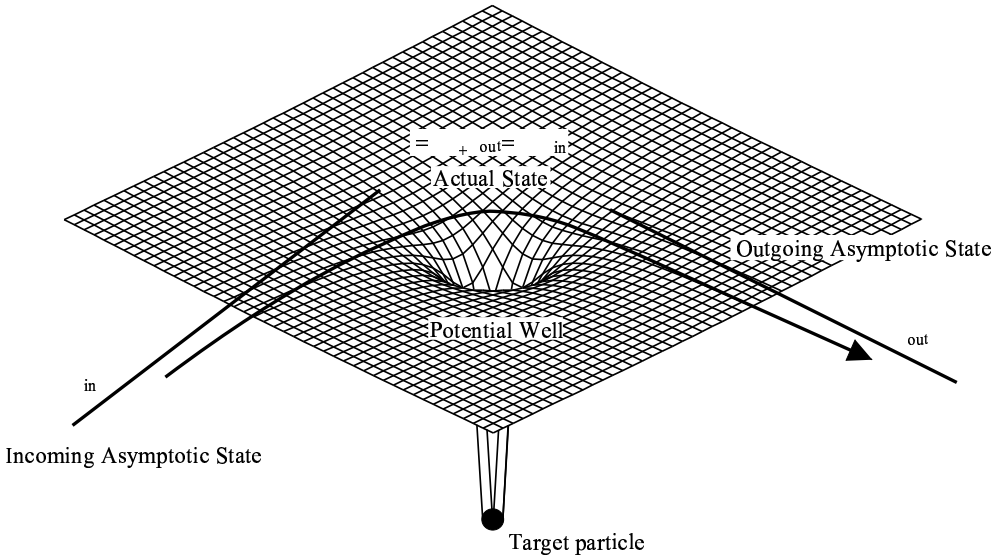


Figure 4.1: A time dependent view of a scattering experiment.

These are defined to be

$$\Omega_{\pm} = \mathrm{s} - \lim_{t \to \mp\infty} e^{iHt} e^{-iH_0 t} E_{M_{\pm}}$$

where $E_{M_{\pm}}$ are the projection operators onto $M_{\pm}$ and ensures that the wave operators are defined everywhere on the Hilbert space. The projection operators exist because the $M_{\pm}$ are closed (as are the $R_{\pm}$) [38]. Although $e^{iHt}$ and $e^{-iH_0 t}$ are unitary operators, the $\Omega_{\pm}$ are in general not unitary. However, it is easy to see that $\Omega_{\pm}$ maps $M_{\pm}$ isometrically onto $R_{\pm}$ and $M_{\pm}^{\perp}$ to $\{0\}$. Such an operator is termed a *partial isometry* (these include as special cases, unitary, isometric and projection operators, see [20] for a discusssion). It is not hard to show that because $\Omega_{\pm}$ is partially isometric from $M_{\pm}$ onto $R_{\pm}$ (just as a unitary operator is isometric from the Hilbert

space onto itself), $\Omega_\pm^\dagger$ is a partial isometry from $R_\pm$ onto $M_\pm$ which behaves somewhat like an inverse. Specifically, we have that $\Omega_\pm\Omega_\pm^\dagger = E_{R_\pm}$ and $\Omega_\pm^\dagger\Omega_\pm = E_{M_\pm}$.

Another important property of the wave operators is that they satisfy the *intertwining relations* [3]:

$$\Omega_\pm E^{H_0}(B) = E^H(B)\Omega_\pm \quad \text{so} \quad \Omega_\pm H_0\Psi = H\Omega_\pm\Psi \quad \forall\Psi\in\mathscr{D}_{H_0} \tag{4.6}$$

where $E^{H_0}(B)$ and $E^H(B)$ are the spectral measures of $H_0$ and $H$ respectively.

We will now define the *scattering operator* $S = \Omega_-^\dagger\Omega_+$. To see why, we first establish that $S$ commutes with the free Hamiltonian. From the intertwining relations, $\Omega_\pm E^{H_0}(B) = E^H(B)\Omega_\pm$ so $E^{H_0}(B)\Omega_\pm^\dagger = \Omega_\pm^\dagger E^H(B)$ so

$$E^{H_0}(B)S = E^{H_0}(B)\Omega_-^\dagger\Omega_+ = \Omega_-^\dagger E^H(B)\Omega_+ = \Omega_-^\dagger\Omega_+ E^{H_0}(B) = SE^{H_0}(B).$$

Now, for any $\Psi\in R_+\cap R_-$ (so both incoming and outgoing asymptotic states, $\Psi_{in}(t)$ and $\Psi_{out}(t)$ exist), we have $\Omega_+\Psi_{in}(0) = \Psi(0) = \Omega_-\Psi_{out}(0)$. Multiplying on the left by $\Omega_-^\dagger$ then gives $S\Psi_{in}(0) = \Omega_-^\dagger\Omega_+\Psi_{in}(0) = \Omega_-^\dagger\Omega_-\Psi_{out}(0) = E_{M_-}\Psi_{out}(0) = \Psi_{out}(0)$ so

$$S\Psi_{in}(t) = Se^{-iH_0t}\Psi_{in}(0) = e^{-iH_0t}S\Psi_{in}(0) = e^{-iH_0t}\Psi_{out}(0) = \Psi_{out}(t).$$

Thus, $S$ takes an incoming state and maps it to the outgoing state. Since the incoming state is usually known and the outgoing state is what we measure, we can see just how fundamental the scattering operator is!

### 4.2.3 Asymptotic Completeness

There is also another condition that we would like a scattering theory to possess. A scattering theory is called *asymptotically complete* if the quantum states with incoming asymptotes are precisely those with outgoing asymptotes, and that these states together with the bound states (which obviously do not satisfy the asymptotic condition) span the entire Hilbert space. That is, $R_+ = R_- = R$ and $R\oplus B$ (where $B$ is the subspace spanned by the bound states) is the whole Hilbert space. In physical terms, this means that the quantum states of the system have to be either bound states or scattering states (or a superposition of the two). Asymptotic completeness is *extremely* hard to verify mathematically. For results concerning classes of potentials for which asymptotic completeness holds in the above sense, see [3], [11] and [37]. [37] also gives an example of a potential for which the Møller wave operators exist (as defined above) but do not give rise to an asymptotically complete theory ($R_+\neq R_-$). However, there are general results proving that for any potential decaying faster than $r^{-1}$, there exists an asymptotically complete (two-body) scattering theory (though not necessarily the one we are discussing, see section 4.5) [23]. We shall therefore assume completeness hereafter.

An immediate consequence of asymptotic completeness is that since $\Omega_+$ maps $M_+$ to $R$ isometrically and $\Omega_-^\dagger$ maps $R$ to $M_-$ isometrically, $S = \Omega_-^\dagger\Omega_+$ maps $M_+$ to $M_-$ isometrically. In the case where $M_+ = M_- = M$ (so any state which represents an incoming asymptote can also represent an outgoing asymptote and vice-versa - this is reasonable if the system is symmetric under time-reversal), we see that the restriction of $S$ to $M$ is unitary. Therefore, for every incoming state, there is an outgoing state with the same norm. This means that the system conserves probability - any particle going into the system must come out again somewhere. It can be shown for instance, that if $V(r)$ is a square-integrable function then $M_+ = M_-$ is the entire Hilbert space, and so $S$ is unitary and probability is conserved [3].

We can also now see that the fact that $S$ commutes with $H_0$ has the physical interpretation that the scattering experiment conserves energy. This is easily seen by comparing the expectation values (section 1.2.6) of the energies of the incoming and outgoing states. Since these states are free, the relevant energy operator is the free Hamiltonian so we have:

$$\begin{aligned}\langle E_{out}\rangle &= \langle\Psi_{out}, H_0\Psi_{out}\rangle = \langle S\Psi_{in}(0), H_0 S\Psi_{in}(0)\rangle \\ &= \langle S\Psi_{in}(0), SH_0\Psi_{in}(0)\rangle = \langle\Psi_{in}(0), H_0\Psi_{in}(0)\rangle = \langle E_{in}\rangle\end{aligned}$$

using the unitarity of $S$.

## 4.3 Time Independent Scattering Theory

The time dependent theory discussed above does not correspond to the way that scattering theory was originally formulated. Historically, the scattering states were treated as stationary states just as bound states usually are, even though it is clear that in scattering the initial wavefunction and the final wavefunction are different. This is the time independent approach and while it gives the correct answers, it was not clear why such a treatment worked. In a sense then, the time dependent theory was developed in order to justify the time independent theory. The time dependent theory however has the disadvantage that it is not obvious how to actually calculate the $S$ operator. The time independent theory on the other hand, furnishes several equations which are useful for calculation purposes. The scattering experiment depicted in figure 1.1 is a time-independent model.

### 4.3.1 The Møller Wave Operators Again

We begin by defining operators $\Omega_{\pm\varepsilon}$ ($\varepsilon > 0$) which are independent of time ($t$):

$$\begin{aligned}\langle f, \Omega_{-\varepsilon} g\rangle &= \varepsilon \int_0^\infty e^{-\varepsilon t} \left\langle f, e^{iHt} e^{-iH_0 t} g\right\rangle dt, \\ \langle f, \Omega_{+\varepsilon} g\rangle &= \varepsilon \int_{-\infty}^0 e^{\varepsilon t} \left\langle f, e^{iHt} e^{-iH_0 t} g\right\rangle dt.\end{aligned}$$

It is easy to show that the integrals on the right are continuous linear functionals so the operators $\Omega_{\pm\varepsilon}$ are well-defined with $\|\Omega_{\pm\varepsilon}\| \leqslant 1$.

As the symbol we have given them suggests, these operators are related to the Møller wave operators. In fact we have [38] that $\Omega_\pm = \mathrm{w}-\lim_{\varepsilon\to 0^+} \Omega_{\pm\varepsilon} E_{M_\pm}$. Since $\|\Omega_{\pm\varepsilon}\| \leqslant 1$ however, we can appeal to lemma 5 to conclude that convergence is strong also. That is,

$$\Omega_\pm = \mathrm{s}-\lim_{\varepsilon\to 0^+} \Omega_{\pm\varepsilon} E_{M_\pm}. \tag{4.7}$$

This is the time independent definition of the Møller wave operators. Here $\varepsilon$ is just a parameter with no physical meaning. We shall see its importance later.

We will also need $\Omega_\pm^\dagger$ in the next section. However, adjointing is not strongly continuous [20] so we cannot immediately take the adjoint into the strong limit. But, adjointing is weakly continuous [20] so we can write

$$\Omega_\pm^\dagger = \mathrm{w}-\lim_{\varepsilon\to 0^+} E_{M_\pm} \Omega_{\pm\varepsilon}^\dagger \quad \Rightarrow \quad \Omega_\pm^\dagger E_{R_\pm} = \mathrm{w}-\lim_{\varepsilon\to 0^+} E_{M_\pm} \Omega_{\pm\varepsilon}^\dagger E_{R_\pm}$$

since multiplication is separately weakly continuous. By definition, $\Omega_\pm^\dagger E_{R_\pm} = \Omega_\pm^\dagger$ since $\Omega_\pm^\dagger$ is a partial isometry from $R_\pm$ to $M_\pm$ and we have $\left\|E_{M_\pm}\Omega_{\pm\varepsilon}^\dagger E_{R_\pm} f\right\| \leqslant \left\|E_{R_\pm} f\right\| = \left\|\Omega_\pm^\dagger E_{R_\pm} f\right\|$. Thus, lemma 5 implies that

$$\Omega_\pm^\dagger = \Omega_\pm^\dagger E_{R_\pm} = \mathrm{s}-\lim_{\varepsilon\to 0^+} E_{M_\pm} \Omega_{\pm\varepsilon}^\dagger E_{R_\pm}. \tag{4.8}$$

### 4.3.2 The Hilbert Space Lippmann-Schwinger Equations

To continue we will need to consider *vector integrals.* These generalise the usual functional integration by allowing vector-valued integrands. Consider the definition of $\Omega_{+\varepsilon}$ :

$$\langle f, \Omega_{+\varepsilon} g\rangle = \varepsilon \int_{-\infty}^0 e^{\varepsilon t} \left\langle f, e^{iHt} e^{-iH_0 t} g\right\rangle dt.$$

We can think of this as the limit of a sequence of integral functionals which converge in the weak topology. However, lemma 5 can again be used to infer that convergence is also strong. To this end, we write

$$\Omega_{+\varepsilon} g = \varepsilon \int_{-\infty}^0 e^{\varepsilon t} e^{iHt} e^{-iH_0 t} g dt$$

where the vector integral is defined in a Riemann sense as the limit of partial sums. It can be shown that many of the simple rules of integration carry over to this more general case. A useful result concerning vector integrals is the following [3].

**Lemma 27** *Let A be self-adjoint and Imz* $\neq 0$. *Then,*

$$\begin{aligned} (z-A)^{-1} f &= -i\int_0^\infty e^{izt} e^{-iAt} f\,dt \quad \textit{when } Imz > 0, \\ \textit{and} \quad (z-A)^{-1} f &= i\int_{-\infty}^0 e^{izt} e^{-iAt} f\,dt \quad \textit{when } Imz < 0. \end{aligned}$$

Now, choose a $\delta > 0$ and partition $[-\delta,\delta]$ according to $-\delta = \lambda_0 < \lambda_1' \leqslant \lambda_1 < \ldots \leqslant \lambda_{n-1} < \lambda_n' \leqslant \lambda_n = \delta$, letting $\nu = \max|\lambda_n - \lambda_{n-1}|$. Following [3], we approximate $\Omega_{+\varepsilon} g$ on $[-\delta,\delta]$ by

$$J_\nu g = \varepsilon \int_{-\infty}^0 e^{\varepsilon t} e^{iHt} \sum_{k=1}^n e^{-i\lambda_k' t} \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g\,dt$$

where we have used a partial sum approximation of the spectral representation for $e^{-iH_0 t}$ :

$$\int_{\mathbb{R}^3} e^{-i\lambda t}\, dE_\lambda^{H_0} \approx \sum_{k=1}^n e^{-i\lambda_k' t} \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right).$$

We therefore have (since $e^{iHt}$ is unitary)

$$\begin{aligned} &\left\|\Omega_{+\varepsilon} E^{H_0}([-\delta,\delta])\, g - J_\nu g\right\| \\ \leqslant\ & \varepsilon \int_{-\infty}^0 e^{\varepsilon t} \left\| e^{-iH_0 t} E^{H_0}([-\delta,\delta])\, g - \sum_{k=1}^n e^{-i\lambda_k' t} \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g \right\| dt. \end{aligned}$$

Now, the integrand is converging to 0 as $\nu \to 0^+$ and is dominated by $2e^{\varepsilon t}\|g\|$ since

$$\left\| \sum_{k=1}^n e^{-i\lambda_k' t} \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g \right\|^2 = \sum_{k=1}^n \left\| \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g \right\|^2 = \left\| E^{H_0}([-\delta,\delta])\, g \right\|^2 \leqslant \|g\|^2.$$

Thus by dominated convergence, $J_\nu \to \Omega_{+\varepsilon} E^{H_0}([-\delta,\delta])$ strongly as $\nu \to 0^+$. But, using lemma 27, we can rewrite $J_\nu$ as:

$$\begin{aligned} J_\nu g &= \varepsilon \sum_{k=1}^n \int_{-\infty}^0 e^{i\left(-\lambda_k' - i\varepsilon\right)t} e^{iHt} \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g\,dt \\ &= \varepsilon \sum_{k=1}^n \int_0^\infty e^{i\left(\lambda_k' + i\varepsilon\right)t} e^{-iHt} \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g\,dt \\ &= i\varepsilon \sum_{k=1}^n \left(\lambda_k' + i\varepsilon - H\right)^{-1} \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g \\ &= i\varepsilon \sum_{k=1}^n G\left(\lambda_k' + i\varepsilon\right) \left(E_{\lambda_k}^{H_0} - E_{\lambda_{k-1}}^{H_0}\right) g \end{aligned}$$

since $\varepsilon > 0$. This looks suspiciously like a partial sum approximation to an integral over $[-\delta,\delta]$ with an operator-valued integrand. Such an integral is often termed a spectral integral and some of its properties are established in [3] and [38]. We write therefore

$$J_\nu \to i\varepsilon \int_{-\delta}^{\delta} G(\lambda + i\varepsilon)\, dE_\lambda^{H_0} \text{ strongly as } \nu \to 0^+.$$

From this then, we have by uniqueness of limits:

$$\begin{aligned} \Omega_{+\varepsilon} &= \operatorname*{s-lim}_{\delta\to\infty} \Omega_{+\varepsilon} E^{H_0}([-\delta,\delta]) = \operatorname*{s-lim}_{\delta\to\infty} i\varepsilon \int_{-\delta}^{\delta} G(\lambda + i\varepsilon)\, dE_\lambda^{H_0} \\ &= i\varepsilon \int_{-\infty}^{\infty} G(\lambda + i\varepsilon)\, dE_\lambda^{H_0} \end{aligned}$$

where the improper integral is defined as the strong limit of proper ones.

A similar derivation gives $\Omega_{-\varepsilon} = -i\varepsilon \int_{-\infty}^{\infty} G(\lambda - i\varepsilon)\, dE_\lambda^{H_0}$. Using equation 4.7, we get the characterisation:

$$\Omega_\pm = \mathrm{s}-\lim_{\varepsilon\to 0^+} \pm i\varepsilon \left[\int_{\mathbb{R}^3} G(\lambda \pm i\varepsilon)\, dE_\lambda^{H_0}\right] E_{M_\pm}. \tag{4.9}$$

We can now derive a most fundamental equation for $\Omega_\pm$ with the help of the following lemma [38].

**Lemma 28** *If $A$ is self-adjoint with spectral function $E_\lambda^A$ and if $H(\lambda)$ is a uniformly bounded operator valued function of $\lambda$ then*

$$\int_{\mathbb{R}^3} H(\lambda)\,(A-\lambda)\, dE_\lambda^A = 0.$$

We write

$$\begin{aligned} \pm i\varepsilon G(\lambda \pm i\varepsilon) &= \pm i\varepsilon\,(\lambda \pm i\varepsilon - H)^{-1} = \frac{\pm i\varepsilon}{\lambda \pm i\varepsilon - H} \\ &= \frac{(\lambda \pm i\varepsilon - H) + (H-\lambda)}{\lambda \pm i\varepsilon - H} = I + \frac{H-\lambda}{\lambda \pm i\varepsilon - H} \end{aligned}$$

which holds rigorously (no domain questions) since the operator functions are in each case bounded ($\varepsilon > 0$). Therefore, we have using lemma 28,

$$\begin{aligned} \Omega_\pm &= \mathrm{s}-\lim_{\varepsilon\to 0^+} \left[\int_{\mathbb{R}^3} I + G(\lambda \pm i\varepsilon)\,(H-\lambda)\, dE_\lambda^{H_0}\right] E_{M_\pm} \\ &= E_{M_\pm} + \mathrm{s}-\lim_{\varepsilon\to 0^+} \left[\int_{\mathbb{R}^3} G(\lambda \pm i\varepsilon)\,(H-H_0)\, dE_\lambda^{H_0}\right] E_{M_\pm} \\ \Rightarrow \Omega_\pm &= E_{M_\pm} + \mathrm{s}-\lim_{\varepsilon\to 0^+} \left[\int_{\mathbb{R}^3} G(\lambda \pm i\varepsilon) V\, dE_\lambda^{H_0}\right] E_{M_\pm}. \end{aligned} \tag{4.10}$$

Applying this to an asymptotic state $f \in M_{\pm,}$ we finally then get the *solution-type Lippmann Schwinger equations in Hilbert space*:

$$f_\pm = f + \mathrm{s}-\lim_{\varepsilon\to 0^+} \left[\int_{\mathbb{R}^3} G(\lambda \pm i\varepsilon) V\, dE_\lambda^{H_0}\right] f. \tag{4.11}$$

We see that this equation gives the actual states of the system $f_\pm = \Omega_\pm f$ in terms of the asymptotic state $f$, the potential $V$, the spectral function of $H_0$, and the full Green's operator $G(\lambda \pm i\varepsilon)$ which is unknown. Recalling that $G(E) = (E-H)^{-1}$ where $E$ represents the energy of the system, we also see that the role of the $\varepsilon$ is that of an *imaginary* energy in the Green's operator. Taking the limit as the energy becomes real from above will thus give $f_+$ which corresponds to treating $f$ as an incoming state. Taking the limit as the energy becomes real from below corresponds to treating $f$ as an outgoing state.

Reflecting on this derivation, however, we can see that when introducing partitions and defining the approximating operator $J_v$, we could very well have chosen to approximate the function $e^{iHt}$ :

$$\int_{\mathbb{R}^3} e^{i\lambda t}\, dE_\lambda^H \approx \sum_{k=1}^{n} e^{i\lambda_k' t}\left(E_{\lambda_k}^H - E_{\lambda_{k-1}}^H\right).$$

Instead of deriving $\Omega_{\pm\varepsilon} = \pm i\varepsilon \left[\int_{\mathbb{R}^3} G(\lambda \pm i\varepsilon)\, dE_\lambda^{H_0}\right]$, then, we would find (respecting the non-commutativity of operator multiplication):

$$\Omega_{\pm\varepsilon} = \mp i\varepsilon \int_{\mathbb{R}^3} \left[dE_\lambda^H\right] \{G_0(\lambda \mp i\varepsilon)\}$$

where the Green's operator is still being integrated but in the approximating partial sums, the spectral functions are pre-multiplied. We can however derive [38] that

$$\begin{aligned}\Omega_{\pm\varepsilon}^{\dagger} &= \pm i\varepsilon\int_{\mathbb{R}^3} G_0(\lambda\pm i\varepsilon)\,dE_\lambda^H = I-\int_{\mathbb{R}^3} G_0(\lambda\pm i\varepsilon)(\lambda-H_0)\,dE_\lambda^H \\ &= I-\int_{\mathbb{R}^3} G_0(\lambda\pm i\varepsilon)V\,dE_\lambda^H\end{aligned}$$

$$\begin{aligned}\Rightarrow\quad \Omega_{\pm}^{\dagger} &= \underset{\varepsilon\to 0^+}{E}{}_{M_\pm}\,\mathrm{s}-\lim\Omega_{\pm\varepsilon}^{\dagger}E_{R_\pm} \\ &= E_{M_\pm}E_{R_\pm}-E_{M_\pm}\mathrm{s}-\lim_{\varepsilon\to 0^+}\left[\int_{\mathbb{R}^3} G_0(\lambda\pm i\varepsilon)V\,dE_\lambda^H\right]E_{R_\pm}. \qquad (4.12)\end{aligned}$$

Therefore, assuming that $M_\pm$ is the whole Hilbert space and applying this to $f_\pm=\Omega_\pm f\in R_\pm$, so that $\Omega_\pm^\dagger f_\pm = f$, we have

$$f = f_\pm - \mathrm{s}-\lim_{\varepsilon\to 0^+}\left[\int_{\mathbb{R}^3} G_0(\lambda\pm i\varepsilon)V\,dE_\lambda^H\right]f_\pm$$

$$\Rightarrow\quad f_\pm = f+\mathrm{s}-\lim_{\varepsilon\to 0^+}\left[\int_{\mathbb{R}^3} G_0(\lambda\pm i\varepsilon)V\,dE_\lambda^H\right]f_\pm \qquad (4.13)$$

which are the *Lippmann-Schwinger equations in Hilbert space*. With these equations, it is the spectral function of $H$ which is not generally known.

### 4.3.3 Eigenfunction Expansions

We are again going to discuss the (three dimensional) Fourier transform and specifically the function

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}},$$

which we introduced as the free plane wave in section 1.2.4. $\phi_{\mathbf{k}}(\mathbf{r})$ can be thought of as an *eigenfunction* of the free Hamiltonian $H_0$ in that $H_0\supseteq -\nabla^2$ (in three dimensions) and $-\nabla^2\phi_{\mathbf{k}}(\mathbf{r})=k^2\phi_{\mathbf{k}}(\mathbf{r})$. Because $\phi_{\mathbf{k}}(\mathbf{r})$ is not square-integrable, it is of course not an eigenvector. In fact, we know that $H_0$ has no point spectrum and hence no eigenvectors (section 3.3.1). However, it is reasonable to associate $\phi_{\mathbf{k}}(\mathbf{r})$ with the point $k^2$ of the continuous spectrum of $H_0$ (which is non-negative) because we can construct a sequence of square-integrable functions which 'approximate' $\phi_{\mathbf{k}}(\mathbf{r})$ in some sense and which show $k^2$ to be in the continuous spectrum (much as we did in section 3.2.1 for the position operator).

The inverse Fourier transform on $S(\mathbb{R}^3)$ can be written as

$$f(\mathbf{r}) = \int_{\mathbb{R}^3}\widehat{f}(\mathbf{k})\,\phi_{\mathbf{k}}(\mathbf{r})\,d\mathbf{r}$$

For comparison we recall (section 1.2.1) that given any orthonormal basis $\{e_n\}$ of $L^2(\mathbb{R}^3)$, we can expand any $f$ as in equation 1.2:

$$f(\mathbf{r}) = \sum_{n=1}^{\infty}\langle e_n, f\rangle\, e_n(\mathbf{r}).$$

We now see that the inverse Fourier transform can be thought of as an expansion of the function $f(\mathbf{r})$ in terms of the $\phi_{\mathbf{k}}(\mathbf{r})$ and with weightings $\widehat{f}(\mathbf{k})$. This is a simple example of what is called an *eigenfunction expansion*.

A fundamental problem in scattering theory is showing that the eigenfunctions of the full Hamiltonian $H\supseteq -\nabla^2+V(\mathbf{r})$, which may be associated with the continuous spectrum, have

a similar eigenfunction expansion property. Namely, these eigenfunctions, called *distorted plane waves* and denoted by $\phi_{\mathbf{k}}^{\pm}(\mathbf{r})$, satisfy

$$f_{\pm}(\mathbf{r}) = (\Omega_{\pm} f)(\mathbf{r}) = \int_{\mathbb{R}^3} \widehat{f}(\mathbf{k})\, \phi_{\mathbf{k}}^{\pm}(\mathbf{r})\, d\mathbf{k} \tag{4.14}$$

for every $f \in M_{\pm} \cap S(\mathbb{R}^3)$. We shall not justify this expansion. Proofs under conditions on $V(\mathbf{r})$ may be found in [3], [38] or [41].

We will use these particular eigenfunction expansions to rewrite the time independent operator equations in terms of the eigenfunctions $\phi_{\mathbf{k}}(\mathbf{r})$ and $\phi_{\mathbf{k}}^{\pm}(\mathbf{r})$. These will not only be more amenable to solution than their Hilbert space counterparts but it turns out that the quantities of interest are more directly related to the eigenfunctions than the actual quantum states. We shall elaborate on this later.

There is one more property of the free plane waves that we need. Recalling that $H_0 = p^2 = p_x^2 + p_y^2 + p_z^2$ where $p_x$, $p_y$ and $p_z$ are the three momentum operators, and equation 3.3 we have for any set $B \subseteq \mathbb{R}^3$,

$$\begin{aligned} \left[E^{H_0}(B) f\right]\hat{}\,(\mathbf{k}) &= \left[\chi_B(H_0) f\right]\hat{}\,(\mathbf{k}) = \left[\chi_B\left(p^2\right) f\right]\hat{}\,(\mathbf{k}) \\ &= \left[\chi_{\sqrt{B}}(p) f\right]\hat{}\,(\mathbf{k}) = \chi_{\sqrt{B}}(\mathbf{k})\, \widehat{f}(\mathbf{k}) \end{aligned}$$

where $\chi$ are characteristic functions and $\sqrt{B} = \left\{(\lambda_1, \lambda_2, \lambda_3) : \left(\lambda_1^2, \lambda_2^2, \lambda_3^2\right) \in B\right\}$. Inverting the Fourier transform, we get

$$\left[E^{H_0}(B) f\right](\mathbf{r}) = \int_{\mathbb{R}^3} \chi_{\sqrt{B}}(\mathbf{k})\, \widehat{f}(\mathbf{k})\, \phi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k} = \int_{\sqrt{B}} \widehat{f}(\mathbf{k})\, \phi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k}. \tag{4.15}$$

We can show something similar for distorted plane waves using the intertwining relations (equation 4.6):

$$\left[E^H(B) f_{\pm}\right](\mathbf{r}) = \left[E^H(B)\Omega_{\pm} f\right](\mathbf{r}) = \left[\Omega_{\pm} E^{H_0}(B) f\right](\mathbf{r}) = \left[E^{H_0}(B) f\right]_{\pm}(\mathbf{r}).$$

Thus, the eigenfunction expansion for distorted plane waves gives

$$\begin{aligned} \left[E^H(B) f_{\pm}\right](\mathbf{r}) &= \int_{\mathbb{R}^3} \left[E^{H_0}(B) f\right]\hat{}\,(\mathbf{k})\, \phi_{\mathbf{k}}^{\pm}(\mathbf{r})\, d\mathbf{k} \\ &= \int_{\mathbb{R}^3} \chi_{\sqrt{B}}(\mathbf{k})\, \widehat{f}(\mathbf{k})\, \phi_{\mathbf{k}}^{\pm}(\mathbf{r})\, d\mathbf{k} = \int_{\sqrt{B}} \widehat{f}(\mathbf{k})\, \phi_{\mathbf{k}}^{\pm}(\mathbf{r})\, d\mathbf{k}. \end{aligned} \tag{4.16}$$

### 4.3.4 The Lippmann-Schwinger Equations

We will illustrate the technique of eigenfunction expansions by decomposing the Hilbert space Lippmann-Schwinger equations (4.13)

$$f_{\pm} = f + \mathrm{s}-\lim_{\varepsilon \to 0^+} \left[\int_{\mathbb{R}^3} G_0(\lambda \pm i\varepsilon) V dE_{\lambda}^H\right] f_{\pm}$$

into equations for the distorted plane waves $\phi_{\mathbf{k}}^{\pm}(\mathbf{r})$. Let $f \in S(\mathbb{R}^3)$. Expanding $f_{\pm} - f$ gives

$$(f_{\pm} - f)(\mathbf{r}) = \int_{\mathbb{R}^3} \widehat{f}(\mathbf{k}) \left[\phi_{\mathbf{k}}^{\pm}(\mathbf{r}) - \phi_{\mathbf{k}}(\mathbf{r})\right] d\mathbf{k}.$$

To tackle the spectral integral on the right, we introduce a partial sum approximation and restrict the integration range to a finite three dimensional interval which we shall denote by $\mathscr{I} = [a_1, b_1] \times .[a_2, b_2] \times [a_3, b_3]$. Let us partition each $[a_m, b_m]$ into $a_m = \lambda_0^{(m)} < \lambda_1^{(m)\prime} \leqslant \lambda_1^{(m)} < \ldots \leqslant \lambda_{n-1}^{(m)} < \lambda_n^{(m)\prime} \leqslant \lambda_n^{(m)} = b_m$, $(m = 1,2,3)$ with $\nu = \max_{m,n} \left|\lambda_n^{(m)} - \lambda_{n-1}^{(m)}\right|$. If we let $\Lambda_j =$

$\left(\lambda_j^{(1)}, \lambda_j^{(2)}, \lambda_j^{(3)}\right)$ for $j = 1, \ldots n$ and $\lambda_j = \left|\Lambda_j\right|$, then

$$\begin{aligned}
&\left[\int_a^b G_0(\lambda \pm i\varepsilon) V dE_\lambda^H f_\pm\right](\mathbf{r}) \\
&= \lim_{\nu\to 0^+} \sum_{j=1}^n \left[G_0\left(\lambda_j' \pm i\varepsilon\right) V\left(E_{\Lambda_j}^H - E_{\Lambda_{j-1}}^H\right) f_\pm\right](\mathbf{r}) \\
&= \lim_{\nu\to 0^+} \sum_{j=1}^n \int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; \lambda_j' \pm i\varepsilon\right) \left[V\left(E_{\Lambda_j}^H - E_{\Lambda_{j-1}}^H\right) f_\pm\right](\mathbf{r}')\, d\mathbf{r}' \\
&= \lim_{\nu\to 0^+} \sum_{j=1}^n \int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; \lambda_j' \pm i\varepsilon\right) V(\mathbf{r}') \left[\left(E_{\Lambda_j}^H - E_{\Lambda_{j-1}}^H\right) f_\pm\right](\mathbf{r}')\, d\mathbf{r}' \\
&= \lim_{\nu\to 0^+} \sum_{j=1}^n \int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; \lambda_j' \pm i\varepsilon\right) V(\mathbf{r}') \left[\int_{\sqrt{B}} \widehat{f}(\mathbf{k})\, \phi_{\mathbf{k}}^\pm(\mathbf{r}')\, d\mathbf{k}\right] d\mathbf{r}' \\
&= \lim_{\nu\to 0^+} \sum_{j=1}^n \int_{\sqrt{B}} \widehat{f}(\mathbf{k}) \left[\int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; \lambda_j' \pm i\varepsilon\right) V(\mathbf{r}')\, \phi_{\mathbf{k}}^\pm(\mathbf{r}')\, d\mathbf{r}'\right] d\mathbf{k} \\
&= \lim_{\nu\to 0^+} \int_a^b \widehat{f}(\mathbf{k}) \left[\int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; \lambda_j' \pm i\varepsilon\right) V(\mathbf{r}')\, \phi_{\mathbf{k}}^\pm(\mathbf{r}')\, d\mathbf{r}'\right] d\mathbf{k} \\
&= \int_a^b \widehat{f}(\mathbf{k}) \left[\int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; k^2 \pm i\varepsilon\right) V(\mathbf{r}')\, \phi_{\mathbf{k}}^\pm(\mathbf{r}')\, d\mathbf{r}'\right] d\mathbf{k}
\end{aligned}$$

where $\sqrt{B}$ is the set $\left\{\mathbf{k} : \lambda_{j-1} < k^2 \leqslant \lambda_j\right\}$ and we have used equation 4.16. We have also applied Fubini's theorem and dominated convergence and the fact that as the partition size vanishes, $\lambda_{j-1} < k^2 \leqslant \lambda_j$ and $\lambda_{j-1} < \lambda_j' \leqslant \lambda_j$ imply that $\lambda_j' \to k^2$.

Now, it should be clear that these steps can only be justified for certain potentials. To invoke Fubini's theorem, the integrand must be integrable (theorem 2). The $\mathbf{k}$ integration is no trouble as $\widehat{f}(\mathbf{k})$ is of rapid decrease and the $\phi_{\mathbf{k}}^\pm(\mathbf{r}')$ are uniformly bounded. The $\mathbf{r}'$ integration is also finite *for square-integrable potentials* since the $\phi_{\mathbf{k}}^\pm(\mathbf{r}')$ are uniformly bounded and $\|G_0 V\|_1 \leqslant \|G_0(\mathbf{r}')\| \|V(\mathbf{r}')\| < \infty$. Therefore, to justify this derivation, we do require conditions on the potential. Square-integrability will do. A similar argument shows that the same condition on the potential also guarantees that we can apply dominated convergence.

Taking limits as $a \to -\infty$ and $b \to \infty$ then gives

$$\left[\int_{\mathbb{R}^3} G_0(\lambda \pm i\varepsilon) V dE_\lambda^H f_\pm\right](\mathbf{r}) = \int_{\mathbb{R}^3} \widehat{f}(\mathbf{k}) \left[\int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; k^2 \pm i\varepsilon\right) V(\mathbf{r}')\, \phi_{\mathbf{k}}^\pm(\mathbf{r}')\, d\mathbf{r}'\right] d\mathbf{k}$$

so substituting into the Hilbert space Lippmann-Schwinger equations gives

$$\begin{aligned}
&\int_{\mathbb{R}^3} \widehat{f}(\mathbf{k}) \left[\phi_{\mathbf{k}}^\pm(\mathbf{r}) - \phi_{\mathbf{k}}(\mathbf{r})\right] d\mathbf{k} \\
&\qquad = \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}^3} \widehat{f}(\mathbf{k}) \left[\int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; k^2 \pm i\varepsilon\right) V(\mathbf{r}')\, \phi_{\mathbf{k}}^\pm(\mathbf{r}')\, d\mathbf{r}'\right] d\mathbf{k}.
\end{aligned}$$

Since $\widehat{f}$ is arbitrary in a dense subspace of $L^2\left(\mathbb{R}^3\right)$, it follows that the functional relation

$$\phi_{\mathbf{k}}^\pm(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}^3} G_0\left(\mathbf{r}, \mathbf{r}'; k^2 \pm i\varepsilon\right) V(\mathbf{r}')\, \phi_{\mathbf{k}}^\pm(\mathbf{r}')\, d\mathbf{r}' \tag{4.17}$$

holds almost everywhere [38]. These are the *Lippmann-Schwinger equations* for the distorted plane waves, and whilst they do not give the $\phi_{\mathbf{k}}^\pm(\mathbf{r})$ explicitly, they do provide a means of calculating $\phi_{\mathbf{k}}^\pm(\mathbf{r})$ from the known functions $\phi_{\mathbf{k}}(\mathbf{r})$, $G_0\left(\mathbf{r}, \mathbf{r}'; k^2 \pm i\varepsilon\right)$ and $V(\mathbf{r}')$. This last process is sometimes called *extracting the kernel equation*.

### 4.3.5 Another Approach

Consider now the solution type Hilbert space Lippmann-Schwinger equations (4.11):

$$f_{\pm} = f + \mathrm{s}-\lim_{\varepsilon\to 0^+}\left[\int_{\mathbb{R}^3} G(\lambda \pm i\varepsilon) V dE_{\lambda}^{H_0}\right] f.$$

By making an eigenfunction expansion, and extracting the kernels, we arrive at the *solution type Lippmann-Schwinger equations*:

$$\phi_{\mathbf{k}}^{\pm}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^3} G\left(\mathbf{r},\mathbf{r}';k^2 \pm i\varepsilon\right) V\left(\mathbf{r}'\right)\phi_{\mathbf{k}}\left(\mathbf{r}'\right) d\mathbf{r}'. \tag{4.18}$$

These equations give the distorted plane waves $\phi_{\mathbf{k}}^{\pm}(\mathbf{r})$ explicitly unlike the original Lippmann-Schwinger equations. However, they do involve the full Green's function $G\left(\mathbf{r},\mathbf{r}';k^2 \pm i\varepsilon\right)$ which is in general unknown. We do however have a relationship between the full and free Green's operators, namely the second resolvent equation (4.4):

$$G(E) = G_0(E) + G_0(E) V G(E).$$

We can expand this equation by applying it to a function $f \in S\left(\mathbb{R}^3\right)$ and then extract the kernels just as we did in the previous section. We will not however have to make any eigenfunction expansions this time. We have

$$\{[G(E) - G_0(E)] f\}(\mathbf{r}) = \int_{\mathbb{R}^3}\left[G\left(\mathbf{r},\mathbf{r}';E\right) - G_0\left(\mathbf{r},\mathbf{r}';E\right)\right] f\left(\mathbf{r}'\right) d\mathbf{r}'$$

and

$$\begin{aligned}
[G_0(E) V G(E) f](\mathbf{r}) &= \int_{\mathbb{R}^3} G_0\left(\mathbf{r},\mathbf{r}'';E\right)[VG(E) f]\left(\mathbf{r}''\right) d\mathbf{r}'' \\
&= \int_{\mathbb{R}^3} G_0\left(\mathbf{r},\mathbf{r}'';E\right) V\left(\mathbf{r}''\right)[G(E) f]\left(\mathbf{r}''\right) d\mathbf{r}'' \\
&= \int_{\mathbb{R}^3} G_0\left(\mathbf{r},\mathbf{r}'';E\right) V\left(\mathbf{r}''\right)\left[\int_{\mathbb{R}^3} G\left(\mathbf{r}'',\mathbf{r}';E\right) f\left(\mathbf{r}'\right) d\mathbf{r}'\right] d\mathbf{r}'' \\
&= \int_{\mathbb{R}^3} f\left(\mathbf{r}'\right)\left[\int_{\mathbb{R}^3} G_0\left(\mathbf{r},\mathbf{r}'';E\right) V\left(\mathbf{r}''\right) G\left(\mathbf{r}'',\mathbf{r}';E\right) d\mathbf{r}''\right] d\mathbf{r}'.
\end{aligned}$$

Extraction of this equation gives

$$G\left(\mathbf{r},\mathbf{r}';E\right) = G_0\left(\mathbf{r},\mathbf{r}';E\right) + \int_{\mathbb{R}^3} G_0\left(\mathbf{r},\mathbf{r}'';E\right) V\left(\mathbf{r}''\right) G\left(\mathbf{r}'',\mathbf{r}';E\right) d\mathbf{r}'' \tag{4.19}$$

to solve for $G(\mathbf{r},\mathbf{r}';E)$. Again, in the derivation we interchanged the order of integration. To justify this, (Fubini's theorem), we must suppose that the integrand was integrable. However, the integrand involves the unknown $G(\mathbf{r}'',\mathbf{r}';E)$, so it is therefore necessary to assume that this step is justified and later make sure that $G(\mathbf{r}'',\mathbf{r}';E)$ does have the property we require of it.

### 4.3.6 The Transition Operator and the On-Shell T-Matrix

Let us now backtrack into Hilbert space again. Recalling the discussion that led to the Hilbert space Lippmann-Schwinger equations, we derived equation 4.12

$$\Omega_{\pm}^{\dagger} = E_{M_{\pm}} E_{R_{\pm}} - E_{M_{\pm}}\mathrm{s}-\lim_{\varepsilon\to 0^+}\left[\int_{\mathbb{R}^3} G_0(\lambda \pm i\varepsilon) V dE_{\lambda}^{H}\right] E_{R_{\pm}}.$$

This yields a time independent expression for the scattering operator $S = \Omega_{-}^{\dagger}\Omega_{+}$ by noting that $\Omega_{+}^{\dagger}\Omega_{+} = I$ assuming $M_{\pm} = L^2\left(\mathbb{R}^3\right)$. Assuming asymptotic completeness also ($R_{+} = R_{-}$), we have:

$$\begin{aligned}
S - I &= \left(\Omega_{-}^{\dagger} - \Omega_{+}^{\dagger}\right)\Omega_{+} \\
&= \left(\mathrm{s}-\lim_{\varepsilon\to 0^+}\left[\int_{\mathbb{R}^3}\{G_0(\lambda + i\varepsilon) - G_0(\lambda - i\varepsilon)\} V dE_{\lambda}^{H}\right] E_{R_{+}}\right)\Omega_{+}.
\end{aligned}$$

Since $\Omega_+$ maps $M_+ = L^2\left(\mathbb{R}^3\right)$ to $R_+$, we have the relation $E_{R_+}\Omega_+ = \Omega_+$. Using this and the intertwining relations then (equation 4.6) gives

$$\begin{aligned} S-I &= \operatorname*{s-lim}_{\varepsilon\to 0^+}\left[\int_{\mathbb{R}^3}\left\{\frac{1}{\lambda+i\varepsilon-H_0}-\frac{1}{\lambda-i\varepsilon-H_0}\right\}VdE_\lambda^H\right]\Omega_+ \\ &= \operatorname*{s-lim}_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}\frac{-2i\varepsilon}{\left(\lambda-H_0\right)^2+\varepsilon^2}V\Omega_+dE_\lambda^{H_0} \\ \Rightarrow \quad S &= I-\operatorname*{s-lim}_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}\frac{2i\varepsilon}{\left(\lambda-H_0\right)^2+\varepsilon^2}V\Omega_+dE_\lambda^{H_0}. \end{aligned} \tag{4.20}$$

Remembering the important relation $S\Psi_{in} = \Psi_{out}$ (section 4.2.2), this equation asserts that the scattering phenomenon may be decomposed into two parts: a part wherein nothing changes (modelled by the identity operator) and a part wherein the complicated scattering process occurs (modelled by the spectral integral in the above equation). In physical terms, the action of the scattering operator on an incoming asymptote gives the original incoming wave, *unscattered* by the potential, superposed with a complicated wave which represents the actual scattering phenomenon. Since we are actually interested in the scattered wave, we separate this term out by introducing the *transition operator* defined by

$$T = \frac{I-S}{2\pi i}$$

(the factor of $2\pi i$ is just for convenience).

The transition operator therefore corresponds to the process wherein the incoming and outgoing states are quite different - that is, the system has undergone a transition. We have the following characterisation:

$$T = \operatorname*{s-lim}_{\varepsilon\to 0^+}\frac{1}{2\pi i}\int_{\mathbb{R}^3}\frac{2i\varepsilon}{\left(\lambda-H_0\right)^2+\varepsilon^2}V\Omega_+dE_\lambda^{H_0}. \tag{4.21}$$

Let us now apply the method of eigenfunction expansions to this equation in the momentum representation. Let $f \in S\left(\mathbb{R}^3\right)$. Approximating the spectral integral as before (section 4.3.4) and making eigenfunction expansions result in the following relation:

$$\begin{aligned} &\left[\int_{\mathbb{R}^3}\frac{2i\varepsilon}{\left(\lambda-H_0\right)^2+\varepsilon^2}V\Omega_+dE_\lambda^{H_0}f\right]\hat{}\,(\mathbf{k}) \\ &\qquad = \int_{\mathbb{R}^3}\frac{2i\varepsilon}{\left(k'^2-k^2\right)^2+\varepsilon^2}\left[\int_{\mathbb{R}^3}\overline{\phi_{\mathbf{k}}(\mathbf{r})}V(\mathbf{r})\,\phi_{\mathbf{k}'}^+(\mathbf{r})\,d\mathbf{r}\right]\widehat{f}\left(\mathbf{k}'\right)d\mathbf{k}' \end{aligned}$$

where we have assumed $V(\mathbf{r}) \in L^1\left(\mathbb{R}^3\right)$, so we may apply Fubini's theorem. For convenience, we define the *T-matrix* by

$$t\left(\mathbf{k},\mathbf{k}'\right) = \int_{\mathbb{R}^3}\overline{\phi_{\mathbf{k}}(\mathbf{r})}V(\mathbf{r})\,\phi_{\mathbf{k}'}^+(\mathbf{r})\,d\mathbf{r}. \tag{4.22}$$

Then the transition operator has the following action in momentum space:

$$(Tf)\hat{}\,(\mathbf{k}) = \lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}\frac{\varepsilon}{\pi\left[\left(k'^2-k^2\right)^2+\varepsilon^2\right]}t\left(\mathbf{k},\mathbf{k}'\right)\widehat{f}\left(\mathbf{k}'\right)d\mathbf{k}'.$$

The name T-matrix refers to the fact that in the Dirac notation, $t(\mathbf{k},\mathbf{k}')$ is written $\langle\mathbf{k}|\,T\,|\mathbf{k}'\rangle$ which would give the entries of the $T$ operator in matrix form if we treated $|\mathbf{k}'\rangle$ and $\langle\mathbf{k}|$ as orthonormal bases.

Now, it is well known that the functions $(\varepsilon/\pi)\left(x^2+\varepsilon^2\right)^{-1}$ 'approximate' a Dirac delta function as $\varepsilon \to 0^+$. In fact, this can be rigorously justified [37], [14] so we have the result

$$(Tf)\hat{}\,(\mathbf{k}) = \int_{\mathbb{R}^3} \delta\left(k'^2 - k^2\right) t\left(\mathbf{k},\mathbf{k}'\right) \widehat{f}\left(\mathbf{k}'\right) d\mathbf{k}'. \tag{4.23}$$

Thus we have the result that the transition operator is (almost) an integral operator in momentum space. Its kernel however, contains a delta function. The effect of this delta function is to restrict the values the T-matrix $t(\mathbf{k},\mathbf{k}')$ take in the integration to those for which $k'^2 = k^2$. Because $k^2$ is just the energy of the system, this means that the energies are the same so the only contribution to the integral comes from T-matrix elements which conserve energy! For this reason, these T-matrix elements are referred to as *on the energy shell* or as the *on-shell T-matrix*.

### 4.3.7 The $\tau$ Operators and the Off-Shell T-Matrix

There is a third equivalent formulation which can be used to solve the scattering problem. Using a similar method to that used to derive the Hilbert space Lippmann-Schwinger equations in section 4.3.2, the following equation for the transtition operator may be derived [3]:

$$T = \mathrm{s}-\lim_{\varepsilon\to 0^+} \mathrm{s}-\lim_{\eta\to 0^+} \int_{\mathbb{R}^3} \frac{\varepsilon}{\pi\left[(\lambda - H_0)^2 + \varepsilon^2\right]} \left[V + VG(\lambda + i\eta)V\right] dE_\lambda^{H_0}. \tag{4.24}$$

Comparing this with the form of the transition operator derived in the last section, we note that this contains the same operator $(\varepsilon/\pi)\left[(\lambda - H_0)^2 + \varepsilon^2\right]^{-1}$ which produced the delta function in the eigenfunction expansion. However, the operator $V + VG(\lambda + i\eta)V$, might by the same reasoning give rise to something like the T-matrix but without the delta function. We will see in the next chapter that it is very convenient to have integral operators with 'smooth' kernels (that is, without delta functions). Therefore we define the operators

$$\tau(E) = V + VG(E)V \tag{4.25}$$

whenever $\mathrm{Im}E \neq 0$ and assume that the $\tau$ operators are integral operators in momentum space:

$$\left[\tau(E)\, f\right]\hat{}\,(\mathbf{k}) = \int_{\mathbb{R}^3} \tau\left(\mathbf{k},\mathbf{k}';E\right) \widehat{f}\left(\mathbf{k}'\right) d\mathbf{k}'.$$

This assertion can be proven similarly to the case of the full Green's operator $G(E)$, which will be proven in section 5.2.2.

Now, if we proceed as usual with the eigenfunction expansion of equation 4.24 with these assumptions, we get

$$(Tf)\hat{}\,(\mathbf{k}) = \lim_{\varepsilon\to 0^+} \lim_{\eta\to 0^+} \int_{\mathbb{R}^3} \frac{\varepsilon}{\pi\left[\left(k'^2 - k^2\right)^2 + \varepsilon^2\right]} \tau\left(\mathbf{k},\mathbf{k}';k'^2 + i\eta\right) \widehat{f}\left(\mathbf{k}'\right) d\mathbf{k}'.$$

Comparing with the result of the last section then, and assuming that $\tau\left(\mathbf{k},\mathbf{k}';k'^2 + i\eta\right)$ is such that the $\eta$-limit may be brought into the integral, we see that

$$t\left(\mathbf{k},\mathbf{k}'\right) = \lim_{\eta\to 0^+} \tau\left(\mathbf{k},\mathbf{k}';k'^2 + i\eta\right). \tag{4.26}$$

The functions $\tau\left(\mathbf{k},\mathbf{k}';k'^2 + i\eta\right)$ are sometimes referred to as the *off-shell T-matrix* for not only do they not conserve energy but they are also defined for complex energies through the parameter $k'^2 + i\eta$. These functions may be calculated by performing an eigenfunction expansion on equation 4.25 if the full Green's function is known. Generally however, we can proceed as follows.

Using the second resolvent equation, we have

$$\begin{aligned} G(E)V &= G_0(E)V + G_0(E)VG(E)V = G_0(E)\left[V + VG(E)V\right] = G_0(E)\,\tau(E) \\ &\Rightarrow \quad \tau(E) = V + VG_0(E)\,\tau(E). \end{aligned} \tag{4.27}$$

An eigenfunction expansion of this equation gives

$$\tau\left(\mathbf{k},\mathbf{k}';E\right)=\widehat{V}\left(\mathbf{k}-\mathbf{k}'\right)+\int_{\mathbb{R}^3}\frac{\widehat{V}\left(\mathbf{k}-\mathbf{k}''\right)}{E-k''^2}\tau\left(\mathbf{k}'',\mathbf{k}';E\right)d\mathbf{k}'' \tag{4.28}$$

where $\widehat{V}\left(\mathbf{k}-\mathbf{k}'\right)=\int_{\mathbb{R}^3}\overline{\phi_{\mathbf{k}}\left(\mathbf{r}\right)}V\left(\mathbf{r}\right)\phi_{\mathbf{k}'}\left(\mathbf{r}\right)d\mathbf{r}$ is the Fourier transform of the potential $V\left(\mathbf{r}\right)$. This is again an integral equation which must be solved to give the off-shell T-matrix.

## 4.4 Summary and Goal

We now finally make the important link back to experiment. Recalling the discussion of section 1.1.2, we suppose that in our scattering experiment we have a beam of particles being fired at a target. Specifically, we assume that the beam has an approximately uniform density of particles. Let $\rho$ be the cross-sectional density of particles in the beam (that is, the number of particles per unit area in the plane perpendicular to the beam). If we have a small detector far from the target which counts the number of particles, $n$, that emerge within a small solid angle $\Delta\Omega$ then the interesting quantity measured by the detector is

$$\frac{n}{\rho\Delta\Omega}.$$

In the limit as $\Delta\Omega$ vanishes, this defines what is called the *differential cross-section*

$$\frac{d\sigma}{d\Omega}=\lim_{\Delta\Omega\to 0^+}\frac{n}{\rho\Delta\Omega}.$$

It should be clear that for very small detectors which are far away from the scattering target, the detector's measurement should be a very good approximation to $d\sigma/d\Omega$. The quantity $\sigma$, defined by integrating over all solid angles:

$$\sigma=\int_\Omega\frac{d\sigma}{d\Omega}d\Omega$$

is known as the *cross-section*. Generally the cross-section and the differential cross-section are dependent on the momentum of the incoming beam of particles.

What needs to be calculated in a theoretical analysis of a scattering problem then, is the differential cross-section. It is well known and shown in any text on scattering theory (eg [46], [45]) that $d\sigma/d\Omega$ is directly related to the *on-shell* T-matrix by

$$\frac{d\sigma}{d\Omega}=4\pi^4\left|t\left(\mathbf{k},\mathbf{k}'\right)\right|^2\quad;\quad\left(k=k'\right) \tag{4.29}$$

although [41] claim that the argument is partially heuristic.

Recalling that we have defined the T-matrix by (4.22)

$$t\left(\mathbf{k},\mathbf{k}'\right)=\int_{\mathbb{R}^3}\overline{\phi_{\mathbf{k}}\left(\mathbf{r}\right)}V\left(\mathbf{r}\right)\phi_{\mathbf{k}'}^+\left(\mathbf{r}\right)d\mathbf{r},$$

we can calculate $t\left(\mathbf{k},\mathbf{k}'\right)$ and hence $d\sigma/d\Omega$ by calculating $\phi_{\mathbf{k}}^+\left(\mathbf{r}\right)$ using the Lippmann-Schwinger equation (4.17):

$$\phi_{\mathbf{k}}^+\left(\mathbf{r}\right)=\phi_{\mathbf{k}}\left(\mathbf{r}\right)+\lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}G_0\left(\mathbf{r},\mathbf{r}';k^2+i\varepsilon\right)V\left(\mathbf{r}'\right)\phi_{\mathbf{k}}^+\left(\mathbf{r}'\right)d\mathbf{r}'$$

which is an integral equation. Alternatively, we can use the second resolvent equation (4.19):

$$G\left(\mathbf{r},\mathbf{r}';E\right)=G_0\left(\mathbf{r},\mathbf{r}';E\right)+\int_{\mathbb{R}^3}G_0\left(\mathbf{r},\mathbf{r}'';E\right)V\left(\mathbf{r}''\right)G\left(\mathbf{r}'',\mathbf{r}';E\right)d\mathbf{r}'',$$

another integral equation, to calculate the full Green's function $G(\mathbf{r},\mathbf{r}';E)$ and then substitute into the solution type Lippmann-Schwinger equation (4.18):

$$\phi_{\mathbf{k}}^{+}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \lim_{\varepsilon\to 0^{+}} \int_{\mathbb{R}^3} G\left(\mathbf{r},\mathbf{r}';k^2+i\varepsilon\right) V\left(\mathbf{r}'\right) \phi_{\mathbf{k}}\left(\mathbf{r}'\right) d\mathbf{r}'.$$

A third option is to solve for the off-shell T-matrix $\tau(\mathbf{k},\mathbf{k}';\lambda)$ using another integral equation (4.28):

$$\tau\left(\mathbf{k},\mathbf{k}';E\right) = \widehat{V}\left(\mathbf{k}-\mathbf{k}'\right) + \int_{\mathbb{R}^3} \frac{\widehat{V}\left(\mathbf{k}-\mathbf{k}''\right)}{E-k''^2} \tau\left(\mathbf{k}'',\mathbf{k}';E\right) d\mathbf{k}''$$

and then calculate the T-matrix immediately by taking limits (4.26):

$$t\left(\mathbf{k},\mathbf{k}'\right) = \lim_{\varepsilon\to 0^{+}} \tau\left(\mathbf{k},\mathbf{k}';k'^2+i\varepsilon\right).$$

## 4.5 The Coulomb Potential

We recall that in deriving the above equations rigorously (and without undue fuss), we have had to make some restrictive assumptions on the potential energy operator. Specifically, we have had to assume that $V(\mathbf{r})$ was integrable and square-integrable over $\mathbb{R}^3$. However, these assumptions exclude the important case of the Coulomb potential between charged particles which has essentially the form

$$V(\mathbf{r}) = \frac{\gamma}{r}$$

($\gamma$ is a constant of proportionality representing the strength of the interaction) and is thus neither integrable or square-integrable. The Coulomb potential is an example of the class of long-range potentials for which the interaction is still significant at large separations.

There are two methods of resolving this problem. The first is to realise that in a real scattering experiment, there are never just two particles. In reality, there are other charged particles which have the effect of shielding the Coulomb interactions. This effectively means that the interaction between two particles becomes effectively zero very quickly as they separate. Mathematically, we can replace the constant $\gamma$ with a function $\gamma(r)$ which agrees with $\gamma$ when $r$ is small but which decays rapidly to zero as $r$ increases. Then the potential is integrable and square-integrable so the equations of this chapter become valid.

The second method is more rigorous and is based on the observation that the asymptotic condition we gave (equation 4.5) is stricter than necessary. In an experiment, one can only measure observable quantities (corresponding to self-adjoint operators), not the actual wavefunction itself. Therefore, we should only claim that a quantum state is converging asymptotically if the expectation values of the relevant observables (momentum, angular momentum, spin, etc...) are converging. Obviously if the wavefunction is asymptotically converging then all the expectation values must converge also, but the converse is not necessarily true! It may thus be possible to define a *weaker* asymptotic condition which allows one to rigorously work with long-range potentials.

This approach was successfully pioneered by Dollard. Because the time independent Schrödinger equation may be solved explicitly for the Coulomb potential, the asymptotic form of the wavefunction can be found (see [35]) and this suggests the form that a *modified wave operator* should take. Dollard introduced the following modified wave operators for the Coulomb case:

$$\Omega_{\pm} = \mathrm{s}-\lim_{t\to\mp\infty} e^{iHt} e^{-i\left[H_0 t+\gamma\ln(4H_0 t)/\left(2\sqrt{H_0}\right)\right]} = \mathrm{s}-\lim_{t\to\mp\infty} e^{iHt} e^{-i\gamma\ln(4H_0 t)/\left(2\sqrt{H_0}\right)} e^{-iH_0 t}$$

and also showed that with these operators, the scattering problem for a Coulomb potential becomes asymptotically complete [3]. The time independent theory can then be formulated accordingly and equations similar to the Lippmann-Schwinger equations can be derived [38]. Discussions of the Coulomb case and general long-range potentials can be found in [3], [35], [38] and [41].

# Chapter 5

# Three-Body Scattering Theory

*"Any formal manipulations that are not obviously wrong are assumed to be correct."*

M L Goldberger and K Watson

## 5.1 Outline

### 5.1.1 Channels

The scattering experiment where three particles are involved is a more complicated, and therefore more interesting, affair. A familiar example of such an experiment is the scattering of an electron off a hydrogen atom. A generalisation of this is when a particle, which we shall call particle 1, scatters off a bound state of two particles, labelled 2 and 3. The bound state will be denoted by $(2,3)$. The complications in three-body scattering arise because there are now different possibilities for the products of the scattering reaction. In the two-body case, the only reaction possible is the following:

$$1 \quad + \quad 2 \quad \rightarrow \quad 1 \quad + \quad 2$$

wherein the first particle scatters of the second and they both separate. Such a reaction is known as *elastic scattering* as the total kinetic energy of the system is conserved. In a three-body experiment, however, it is also possible for the bound state $(2,3)$ to be raised to an excited state $(2,3)^*$ so the kinetic energy of the system is not conserved in the reaction. This is known as *inelastic scattering*, and can occur if the energy of particle 1 is sufficiently high. We also have the possibility that, if the energy is higher still, the bound state may be raised to a continuum state $2+3$ which effectively breaks particles 2 and 3 apart. This is called *ionisation*. Finally, we have the possibility that the incoming particle 1 may "pick up" particle 2 so that the final state is a bound state $(1,2)$ with particle 3 free. This is termed *rearrangement*. Summarising then, in our example of a three-body scattering experiment, there are four possible types of reactions:

$$\begin{array}{lllll}
1 + (2,3) & \rightarrow & 1 + (2,3) & & \text{(elastic scattering)} \\
1 + (2,3) & \rightarrow & 1 + (2,3)^* & & \text{(inelastic scattering)} \\
1 + (2,3) & \rightarrow & 1 + 2 + 3 & & \text{(ionisation)} \\
1 + (2,3) & \rightarrow & (1,2) + 3 & & \text{(rearrangement)}
\end{array}$$

each of which can occur if energetically possible.

Each of these possibilities is termed a reaction *channel* and correspond to a different outcome to the same scattering experiment. Of course, being a quantum system, we should expect the final state of a scattering experiment to be some superposition of all these possibilities, so each channel has a certain probability or likelihood associated with it. We shall see shortly that the two-body scattering theory (which is a one channel theory) discussed in the last chapter

is easily generalised to accomodate the extra complications that this *multi-channel scattering* introduces. As before, we shall be primarily concerned with potentials which decay rapidly, again excluding the Coulomb potential. However, it is still possible to modify the theory (as noted in section 4.5) so that this important case can still be treated (see [12]).

### 5.1.2 Channel Operators

We shall assume that the potential energy operator of the quantum system has the form

$$V(r_1,r_2,r_3) = V_1(|r_2-r_3|) + V_2(|r_1-r_3|) + V_3(|r_1-r_2|) \tag{5.1}$$

where $r_1, r_2,$ and $r_3$ are the position operators for particles $1,2,$ and $3$ respectively. This is therefore just the sum of the possible two-body potentials (it is of course possible to include more general terms [45]). $V_i$ then represents the interaction between particles $j$ and $k$ ($i \neq j \neq k$). We now introduce the *channel Hamiltonians* defined by

$$H_i = H_0 + V_i$$

for $i = 1,2,3$ ($H_0 = p_1^2/2m_1 + p_2^2/2m_2 + p_3^2/2m_3$ as usual where $p_i$ is the momentum operator of particle $i$ and $m_i$ is its mass). If we consider a channel in which particle 1 and the bound state $(2,3)$ move freely, then the Hamiltonian becomes $H_1 = H_0 + V_1$ for large separations, since $V_2$ and $V_3$ decay rapidly. We will call this channel-1. Similarly, $H_2$ represents the "asymptotic Hamiltonian" for channel-2 in which particle 2 is free and $(1,3)$ is bound, etc... For an ionisation channel where all three particles are free, the corresponding Hamiltonian is of course just the free Hamiltonian $H_0$. This will therefore be denoted by channel-0.

We expect that the *asymptotic states* corresponding to channel-$\alpha$ to evolve in time according to

$$\Psi_\alpha(t) = e^{-iH_\alpha t}\Psi_\alpha(0)$$

where $\Psi_\alpha(t)$ is an asymptotic state for which there exists a state $\Psi(t)$ obeying the following *asymptotic condition*:

$$\|\Psi_\alpha(t) - \Psi(t)\| \to 0 \text{ as } t \to \pm\infty.$$

Proceeding as in section 4.2.2, we define

$$M_\pm^\alpha = \left\{ f : \mathrm{s}-\lim_{t\to\mp\infty} e^{iHt}e^{-iH_\alpha t} f \text{ exists} \right\}$$

which are the asymptotic states corresponding to channel-$\alpha$ and are closed subspaces of the Hilbert space. We thus define the channel wave operators

$$\Omega_\pm^\alpha = \mathrm{s}-\lim_{t\to\mp\infty} e^{iHt}e^{-iH_\alpha t}E_{M_\pm^\alpha}$$

where $E_{M_\pm^\alpha}$ are the projection operators onto $M_\pm^\alpha$. These are partial isometries which obviously share the same properties as the two-body wave operators.

We now define the analogue of the scattering operator. Since a system in an initial channel does not have to end up in the same channel, there will exist a scattering operator for every possible combination. Thus, for every incoming channel $\alpha$ and outgoing channel $\beta$, there is a scattering operator

$$S_{\beta\alpha} = \left(\Omega_-^\beta\right)^\dagger \Omega_+^\alpha \tag{5.2}$$

which is such that $S_{\beta\alpha}\Psi_\alpha(t) = \Psi_\beta(t)$ for all asymptotic states $\Psi_\alpha(t) \in M_+^\alpha$ and $\Psi_\beta(t) \in M_-^\beta$ [38].

It is also clear that the time independent definition of the wave operators given in section 4.3.1 can also be generalised to

$$\begin{aligned} \Omega_+^\alpha &= \mathrm{s}-\lim_{\varepsilon\to 0^+} \varepsilon \int_{-\infty}^0 e^{\varepsilon t}e^{iHt}e^{-iH_\alpha t}E_{M_+^\alpha}dt \\ \text{and} \quad \Omega_-^\alpha &= \mathrm{s}-\lim_{\varepsilon\to 0^+} \varepsilon \int_0^\infty e^{-\varepsilon t}e^{iHt}e^{-iH_\alpha t}E_{M_-^\alpha}dt \end{aligned}$$

and that the proof given there that the time independent and dependent definitions are equivalent can be trivially modified to cover this generalisation. Hence, the time independent theory proceeds as before (see [38]). Problems only arise at the eigenfunction expansion stage when we need to apply Fubini's theorem and dominated convergence to extract the kernel equations (section 4.3.4). To do this rigorously, we required the potential to be square-integrable. Unfortunately, this is not true in the three-body case. In fact, because each term of the potential is a function of only two particle coordinates, they cannot be square-integrable in the third coordinate.

It is customary in the physical literature to ignore these irritating technicalities however and assume that the kernel equations are correct (see [35] or [45]) and this view does have some experimental support. These kernel equations are then similar to the Lippmann-Schwinger equations we derived in the last chapter. However, we shall see shortly (after tidying up some of the two body theory) that even if these three body Lippmann-Schwinger equations are correct, they are not entirely satisfactory for calculating the wavefunction or T-matrix and hence the differential cross-sections.

## 5.2 Why Three-Body Scattering Theory is So Hard!

We now wish to examine the equations of scattering theory that we derived in the last chapter. Specifically, we shall be looking at the question of whether or not these equations are actually suitable for determining the quantities of interest. By this we mean, do the equations of scattering theory actually have solutions and if they do, are the solutions unique? Of course from a physical point of view, the answer to both these questions had better be yes, for otherwise these equations are not going to be of much use to us! The point of an integral equation formulation is that the boundary conditions required are implicitly incorporated. If our equations have many solutions then we would have to explicitly apply boundary conditions (which we may not know!) to determine the correct solution. However, with numerical approximations, uniqueness of solution is vital because we have no way of knowing if the solution we have calculated is correct or is it just a 'mish-mash' of many possible solutions. We shall see shortly that these questions can be answered for two-body scattering theory affirmatively using the *Fredholm theory* of integral equations.

### 5.2.1 Compact Operators and Fredholm Theory

We recall that each of the equations we derived to solve the two-body scattering problem was an integral equation. In fact, each had the particular form

$$f(x) = g(x) + \int K(x,y)\, f(y)\, dy \tag{5.3}$$

where $f(x)$ was the unknown function. An equation of this kind in the variable $x$ is known as an *integral equation of the second kind* with dummy variable $y$. The functions $g(x)$ and $K(x,y)$ are known as the *free term* and the *kernel* respectively. Fredholm theory provides sufficient conditions for an equation of this type to have a unique solution. To discuss this however, we shall need to introduce the concept of a compact operator.

There are many equivalent definitions of a compact operator (also known as a *completely continuous operator*). We shall say that an operator $K$ acting on a Hilbert space is *compact* if given any sequence of vectors $(f_n)$ which are bounded ($\sup_n \|f_n\| < \infty$), the sequence $(Kf_n)$ has a convergent subsequence. An important spectral property of compact operators is the following [27]:

**Theorem 29** *If $K$ is a compact operator and $\lambda \in \sigma(K)$ for any $\lambda \neq 0$, then $\lambda \in \sigma_p(K)$. That is, any non-zero value of the spectrum of $K$ is an eigenvalue.*

Let us now reconsider equation 5.3. If we are working in the Hilbert space $L^2(\mathbb{R}^n)$ so $f(x)$ and $g(x)$ can be treated as vectors of this space then we may rewrite this equation in the abstract form

$$f = g + Kf$$

where $K$ is an integral operator (not necessarily self-adjoint) defined by

$$(Kf)(x) = \int K(x,y) f(y)\, dy.$$

This equation is easily seen to have the unique solution

$$f = (I-K)^{-1} g$$

(where $I$ is the identity operator) if $(I-K)^{-1}$ exists and $g \in \mathscr{D}_{(I-K)^{-1}}$. Recalling section 2.4, we note that the first condition will be satisfied if $1 \notin \sigma_p(K)$ and the second condition is only relevant if $1 \in \sigma_c(K)$. This is where compactness comes in. If the operator $K$ is compact, then by theorem 29, $1 \in \sigma(K)$ implies that $1 \in \sigma_p(K)$ so we do not need to worry about the second condition. Therefore, if $K$ is compact, then our integral equation has a unique solution if 1 is not an eigenvalue of $K$. Furthermore, standard Fredholm theory then gives an algorithm for calculating the solution. This may be found in [6] or [44].

To prove that our scattering equations are actually worth solving then, it will be sufficient to show that they involve a compact integral operator which does not have 1 as an eigenvalue. Therefore, we need a test to determine if an integral operator is compact. The following theorem gives a sufficient condition for showing this [39]:

**Theorem 30** *If an integral operator $K$ on $L^2(\mathbb{R}^n)$ has a kernel $K(x,y)$ which is square-integrable ($K(x,y) \in L^2(\mathbb{R}^{2n})$) then $K$ is compact.*

The class of compact operators which can be represented on $L^2(M,\mu)$ for some measurable space $M$ with measure $\mu$, as integral operators with square-integrable kernels is called the *Hilbert-Schmidt class*. We shall also say that the kernel $K(x,y)$ of an integral equation is compact if the integral operator it induces is compact.

### 5.2.2 Tidying up the Two-Body Theory

We now show that the integral equations we derived in the last chapter have the compactness property we would like of them. Recall the second resolvent identity in kernel form (equation 4.19):

$$G(\mathbf{r},\mathbf{r}';E) = G_0(\mathbf{r},\mathbf{r}';E) + \int_{\mathbb{R}^3} G_0(\mathbf{r},\mathbf{r}'';E)\, V(\mathbf{r}'')\, G(\mathbf{r}'',\mathbf{r}';E)\, d\mathbf{r}''.$$

If we treat the variable $\mathbf{r}'$ as a parameter then this equation is an integral equation in the variable $\mathbf{r}$ with dummy variable $\mathbf{r}''$ and kernel $G_0(\mathbf{r},\mathbf{r}'';E)V(\mathbf{r}'')$. Since $\mathrm{Im}E \neq 0$ (section 4.1.2), we have by equation 4.3 that $G_0(\mathbf{r},\mathbf{r}';E) \in L^2(\mathbb{R}^3)$ for every $\mathbf{r}'$ :

$$\int_{\mathbb{R}^3} \left|G_0(\mathbf{r},\mathbf{r}';E)\right|^2 d\mathbf{r} = \frac{1}{8\pi \mathrm{Im}\sqrt{E}}$$

and if $V(\mathbf{r}) \in L^2(\mathbb{R}^3)$ also (as we generally assumed in the last chapter), then the kernel is square-integrable in $L^2(\mathbb{R}^6)$ hence compact by theorem 30:

$$\begin{aligned}\int_{\mathbb{R}^6} \left|G_0(\mathbf{r},\mathbf{r}'';E)\, V(\mathbf{r}'')\right|^2 d\mathbf{r}d\mathbf{r}'' &= \int_{\mathbb{R}^3} \left|V(\mathbf{r}'')\right|^2 \left[\int_{\mathbb{R}^3} \left|G_0(\mathbf{r},\mathbf{r}'';E)\right|^2 d\mathbf{r}\right] d\mathbf{r}'' \\ &= \frac{1}{8\pi \mathrm{Im}\sqrt{E}} \int_{\mathbb{R}^3} \left|V(\mathbf{r}'')\right|^2 d\mathbf{r}'' < \infty.\end{aligned}$$

Therefore, we may treat the second resolvent identity as an integral equation in the Hilbert space $L^2(\mathbb{R}^3)$ with a compact kernel. Thus, $G(\mathbf{r},\mathbf{r}';E)$ exists (in $L^2(\mathbb{R}^3)$) and is unique if 1

is not an eigenvalue of the compact integral operator $G_0(E)V$. Let us suppose then that 1 is an eigenvalue of $G_0(E)V$ so there exists an $f \in L^2(\mathbb{R}^3)$ such that $G_0(E)Vf = f$. This means that

$$(E-H_0)^{-1}Vf = f \quad \Rightarrow \quad Vf = (E-H_0)f \quad \Rightarrow \quad (H_0+V)f = Ef \quad \Rightarrow \quad Hf = Ef$$

so $E$ would be an eigenvalue of the Hamiltonian, contradicting the fact that $H$ is self-adjoint and $\mathrm{Im}E \neq 0$. Therefore 1 is not an eigenvalue of $G_0(E)V$ so $G(\mathbf{r},\mathbf{r}';E)$ exists, is square-integrable in $\mathbf{r}$, and is unique.

In fact, using a little more Fredholm theory, it can be shown that $G(\mathbf{r},\mathbf{r}';E)$ is symmetric in $\mathbf{r}$ and $\mathbf{r}'$ :

$$G(\mathbf{r},\mathbf{r}';E) = G(\mathbf{r}',\mathbf{r};E) \tag{5.4}$$

just as $G_0(\mathbf{r},\mathbf{r}';E)$ is [38]. Therefore we have

$$\int_{\mathbb{R}^3} \left|G(\mathbf{r},\mathbf{r}';E)\right|^2 d\mathbf{r} = \int_{\mathbb{R}^3} \left|G(\mathbf{r}',\mathbf{r};E)\right|^2 d\mathbf{r}' = \int_{\mathbb{R}^3} \left|G(\mathbf{r},\mathbf{r}';E)\right|^2 d\mathbf{r}'$$

and since the first expression is a function of $\mathbf{r}'$ but the last is a function of $\mathbf{r}$, it follows that both are constant (independent of either variable). Using this result we can now finally justify the use of Fubini's theorem in interchanging the order of integration in the eigenfunction expansion of the second resolvent equation (section 4.3.5). Recalling that we needed to show that the integrand of the expression:

$$\int_{\mathbb{R}^3} G_0(\mathbf{r},\mathbf{r}'';E)V(\mathbf{r}'')\left[\int_{\mathbb{R}^3} G(\mathbf{r}'',\mathbf{r}';E)\, f(\mathbf{r}')\, d\mathbf{r}'\right] d\mathbf{r}''$$

was integrable in $\mathbf{r}'$ and $\mathbf{r}''$ for any $f \in S(\mathbb{R}^3)$, we can now see that

$$\begin{aligned}
&\int_{\mathbb{R}^6} \left|G_0(\mathbf{r},\mathbf{r}'';E)V(\mathbf{r}'')G(\mathbf{r}'',\mathbf{r}';E)\, f(\mathbf{r}')\right| d\mathbf{r}'d\mathbf{r}'' \\
&\qquad \leqslant \|f\| \int_{\mathbb{R}^3} \left|G_0(\mathbf{r},\mathbf{r}'';E)V(\mathbf{r}'')\right| \int_{\mathbb{R}^3} \left|G(\mathbf{r}'',\mathbf{r}';E)\right|^2 d\mathbf{r}'d\mathbf{r}'' \\
&\qquad\qquad \leqslant \|f\| \left\|G(\mathbf{r},\mathbf{r}';E)\right\| \int_{\mathbb{R}^3} G_0(\mathbf{r},\mathbf{r}'';E)V(\mathbf{r}'')\, d\mathbf{r}'' \\
&\qquad\qquad\qquad \leqslant \|f\| \left\|G(\mathbf{r},\mathbf{r}';E)\right\| \left\|G_0(\mathbf{r},\mathbf{r}';E)\right\| \|V(\mathbf{r})\| < \infty
\end{aligned}$$

where we have let $\|G(\mathbf{r},\mathbf{r}';E)\|^2 = \int_{\mathbb{R}^3} |G(\mathbf{r},\mathbf{r}';E)|^2\, d\mathbf{r}$ and similarly for $G_0(\mathbf{r},\mathbf{r}';E)$.

This result then proves the claim we made in section 4.1.2 that the full Green's operator was an integral operator with kernel $G(\mathbf{r},\mathbf{r}';E)$. The argument is not circular - we have assumed that the full Green's operator $G(E)$ is an integral operator with kernel $G(\mathbf{r},\mathbf{r}';E)$ that satisfies certain properties (allowing us to use Fubini's theorem). We have shown that if this is all true, then $G(\mathbf{r},\mathbf{r}';E)$ satisfies an integral equation of the second kind and that this equation admits a solution with the right properties. Since there are no contradictions to be found, the solution of our integral equation *is* the kernel of $G(E)$ which is thus an integral operator.

It is also possible to establish that equation 4.28 for the off-shell T-matrix:

$$\tau(\mathbf{k},\mathbf{k}';E) = \widehat{V}(\mathbf{k}-\mathbf{k}') + \int_{\mathbb{R}^3} \frac{\widehat{V}(\mathbf{k}-\mathbf{k}'')}{E-k''^2}\tau(\mathbf{k}'',\mathbf{k}';E)\, d\mathbf{k}''$$

is compact and that this equation has a unique solution using Fredholm theory. The details may be found in [11].

### 5.2.3 A Problem with Computation

Let us now reflect. We have now proven that there is a unique solution to the kernel form of the second resolvent equation. Therefore, by solving this equation and substituting into

the solution type Lippmann Schwinger equations, we have the wavefunction and hence the T-matrix. However, we recall that when substituting $G\left(\mathbf{r},\mathbf{r}';k^2+i\varepsilon\right)$ into the solution type Lippmann-Schwinger equations, we have to take the limit as $\varepsilon\to 0^+$. This is where the computation becomes a bit sloppy. We should not, in general, expect to be able to solve the second resolvent equation analytically so we are restricted to calculating approximate solutions with a computer. But then, to calculate the wavefunction accurately, we must solve the second resolvent equation *many* times (for different $\varepsilon$) in order to take the limit as $\varepsilon\to 0^+$. Clearly it would be better if we could solve an equation wherein this limiting procedure was already incorporated.

Recall the Lippmann-Schwinger equation (4.17):

$$\phi_{\mathbf{k}}^{+}(\mathbf{r})=\phi_{\mathbf{k}}(\mathbf{r})+\lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}G_0\left(\mathbf{r},\mathbf{r}';k^2+i\varepsilon\right)V\left(\mathbf{r}'\right)\phi_{\mathbf{k}}^{+}\left(\mathbf{r}'\right)d\mathbf{r}'.$$

Let us now define the *outgoing free Green's function*:

$$G_0^{+}\left(\mathbf{r},\mathbf{r}';k^2\right)=\lim_{\varepsilon\to 0^+}G_0\left(\mathbf{r},\mathbf{r}';k^2+i\varepsilon\right)=\frac{-1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

for $k$ real. Then, by taking the limit inside the integral, we have

$$\phi_{\mathbf{k}}^{+}(\mathbf{r})=\phi_{\mathbf{k}}(\mathbf{r})+\int_{\mathbb{R}^3}G_0^{+}\left(\mathbf{r},\mathbf{r}';k^2\right)V\left(\mathbf{r}'\right)\phi_{\mathbf{k}}^{+}\left(\mathbf{r}'\right)d\mathbf{r}'. \tag{5.5}$$

To rigorously justify this step, we must assume that the potential satisfies

$$\int_{\mathbb{R}^3}\frac{|V(\mathbf{r}')|}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'<\infty$$

so that dominated convergence may be applied. This will be the case, for instance, if $V(\mathbf{r})$ is continuous everywhere and decays faster than $r^{-2}$.

For such potentials then, we now have a Lippmann-Schwinger equation for which the $\varepsilon$-limit has been absorbed and the energy parameter ($k^2$) is real. However, the kernel of this equation is not square-integrable as $G_0^{+}\left(\mathbf{r},\mathbf{r}';k^2\right)$ is clearly not square-integrable in $\mathbf{r}$. In fact, the free term $\phi_{\mathbf{k}}(\mathbf{r})$ is not a vector from $L^2\left(\mathbb{R}^3\right)$ either so we cannot apply the Hilbert space Fredholm theory discussed in section 5.2.1.

There is, however, a sneaky little trick first discovered by *Rollnik* which allows us to rewrite this equation with a compact kernel for a large class of potentials. We factorise the potential as

$$V(\mathbf{r})=|V(\mathbf{r})|^{1/2}\left[V(\mathbf{r})\right]^{1/2}$$

where $\left[V(\mathbf{r})\right]^{1/2}=|V(\mathbf{r})|^{1/2}sgn\left[V(\mathbf{r})\right]$ (the *sgn* function preserves the sign of $V(\mathbf{r})$ everywhere). Inserting this factorisation into the Lippmann-Schwinger equation and multiplying each side by $\left[V(\mathbf{r})\right]^{1/2}$ gives

$$\begin{aligned}
&\left[V(\mathbf{r})\right]^{1/2}\phi_{\mathbf{k}}^{+}(\mathbf{r})\\
=\;&\left[V(\mathbf{r})\right]^{1/2}\phi_{\mathbf{k}}(\mathbf{r})+\int_{\mathbb{R}^3}\left[V(\mathbf{r})\right]^{1/2}G_0^{+}\left(\mathbf{r},\mathbf{r}';k^2\right)\left|V\left(\mathbf{r}'\right)\right|^{1/2}\left[V\left(\mathbf{r}'\right)\right]^{1/2}\phi_{\mathbf{k}}^{+}\left(\mathbf{r}'\right)d\mathbf{r}'\\
\Rightarrow\quad&\widetilde{\phi_{\mathbf{k}}^{+}}(\mathbf{r})=\widetilde{\phi_{\mathbf{k}}}(\mathbf{r})+\int_{\mathbb{R}^3}\left[V(\mathbf{r})\right]^{1/2}G_0^{+}\left(\mathbf{r},\mathbf{r}';k^2\right)\left|V\left(\mathbf{r}'\right)\right|^{1/2}\widetilde{\phi_{\mathbf{k}}^{+}}\left(\mathbf{r}'\right)d\mathbf{r}'
\end{aligned}\tag{5.6}$$

where we have set $\widetilde{\phi_{\mathbf{k}}^{+}}(\mathbf{r})=\left[V(\mathbf{r})\right]^{1/2}\phi_{\mathbf{k}}^{+}(\mathbf{r})$ and $\widetilde{\phi_{\mathbf{k}}}(\mathbf{r})=\left[V(\mathbf{r})\right]^{1/2}\phi_{\mathbf{k}}(\mathbf{r})$.

For the class of potentials for which $V(\mathbf{r})$ is continuous and decays faster than $r^{-2}$, it is easily checked that $\widetilde{\phi_{\mathbf{k}}^{+}}(\mathbf{r})$ and $\widetilde{\phi_{\mathbf{k}}}(\mathbf{r})$ are square-integrable. Furthermore, the kernel of this equation is compact:

$$\int_{\mathbb{R}^6}\left|\left[V(\mathbf{r})\right]^{1/2}G_0^{+}\left(\mathbf{r},\mathbf{r}';k^2\right)\left|V\left(\mathbf{r}'\right)\right|^{1/2}\right|^2d\mathbf{r}d\mathbf{r}'=\frac{1}{16\pi^2}\int_{\mathbb{R}^6}\frac{|V(\mathbf{r})|\,|V(\mathbf{r}')|}{|\mathbf{r}-\mathbf{r}'|^2}d\mathbf{r}d\mathbf{r}'<\infty$$

for such potentials [3]. It can also be shown that the integral operator with kernel

$$[V(\mathbf{r})]^{1/2} G_0^+(\mathbf{r},\mathbf{r}';k^2) \left|V(\mathbf{r}')\right|^{1/2}$$

does not have 1 as an eigenvalue for *almost every* $k \in \mathbb{R}$ (the set of $k$ for which 1 is an eigenvalue has Lebesgue measure zero) [41]. Therefore, by restricting the potential as above, it can be rigorously shown that the Lippmann-Schwinger equation with the limit implicitly incorporated also provides a suitable method for calculating the wavefunction for a two-body scattering process.

### 5.2.4 The Problem with Three Particles

We are now ready to discuss exactly why the three-body Lippmann-Schwinger equations that we alluded to in section 5.1.2 are not suitable for computing the wavefunction. For every channel $\alpha$, we have defined a channel Hamiltonian $H_\alpha = H_0 + V_\alpha$ which thus gives rise to a *channel Green's operator*:

$$G_\alpha(E) = (E - H_\alpha)^{-1}$$

for $\mathrm{Im}E \neq 0$. It seems reasonable to assume that $G_\alpha(E)$ is an integral operator:

$$[G_\alpha(E) f](\mathbf{R}) = \int_{\mathbb{R}^9} G_\alpha(\mathbf{R},\mathbf{R}';E) f(\mathbf{R}') d\mathbf{R}'$$

where $\mathbf{R} = (\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ refers to the positions of the particles.

Let us suppose that the incoming asymptote of our scattering experiment is in a definite channel $\alpha$, and is described by the (known) wavefunction $\phi_{\mathbf{K}}(\mathbf{R};\alpha)$ where $\mathbf{K} = (\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)$ refers to the momenta of the particles. For instance, in channel 1 where particle 1 is initially free and 2 and 3 are bound, this wavefunction would have the form

$$\phi_{\mathbf{K}}(\mathbf{R};\alpha) = \phi_{\mathbf{k}_1}(\mathbf{r}_1)\chi_{\mathbf{k}_2,\mathbf{k}_3}(\mathbf{r}_2,\mathbf{r}_3)$$

where $\phi_{\mathbf{k}_1}(\mathbf{r}_1)$ is a plane wave and $\chi_{\mathbf{k}_2,\mathbf{k}_3}(\mathbf{r}_2,\mathbf{r}_3)$ is a bound state wavefunction for 2 and 3. The actual wavefunction, denoted by $\phi_{\mathbf{K}}^+(\mathbf{R};\alpha)$, would then obey the following Lippmann-Schwinger equation [45] (for which interchanging the order of integration in the eigenfunction expansion is *not* justified by Fubini's theorem):

$$\phi_{\mathbf{K}}^+(\mathbf{R};\alpha) = \phi_{\mathbf{K}}(\mathbf{R};\alpha) + \int_{\mathbb{R}^9} G_\alpha(\mathbf{R},\mathbf{R}';E) V_\alpha\left(\left|\mathbf{r}'_\beta - \mathbf{r}'_\gamma\right|\right) \phi_{\mathbf{K}}^+(\mathbf{R}';\alpha) d\mathbf{R}' \tag{5.7}$$

where $(\alpha \neq \beta \neq \gamma)$. As in the two-body case, it is only the free Green's function $G_0(\mathbf{R},\mathbf{R}';E)$ which is known. To calculate the channel Green's function, $G_\alpha(\mathbf{R},\mathbf{R}';E)$, we must appeal to another version of the second resolvent equation:

$$G_\alpha(E) = G_0(E) + G_0(E) V_\alpha G_\alpha(E) \tag{5.8}$$

which is in kernel form,

$$G_\alpha(\mathbf{R},\mathbf{R}';E) = G_0(\mathbf{R},\mathbf{R}';E) + \int_{\mathbb{R}^9} G_0(\mathbf{R},\mathbf{R}'';E) V_\alpha\left(\left|\mathbf{r}'_\beta - \mathbf{r}'_\gamma\right|\right) G_\alpha(\mathbf{R}'',\mathbf{R}';E) d\mathbf{R}'' \tag{5.9}$$

where again, $(\alpha \neq \beta \neq \gamma)$. Now, it is immediately apparent that the kernel of this equation cannot be square-integrable in $r_\alpha$ and $r'_\alpha$. Therefore, we cannot conclude that this three-body second resolvent equation is compact. However, in contrast to the last section, we cannot use a trick to rewrite this as a compact equation because the following theorem [35] asserts that this equation is in fact, *not* compact. This is sometimes called the failure of the three-body Lippmann-Schwinger equations.

**Theorem 31** *Suppose that $A$ is a self-adjoint operator with $\sigma_p(A) = \varnothing$ (that is, with a purely continuous spectrum). Then if $K$ is a compact operator that commutes with $A$, $K = 0$, the zero operator.*

Now, we know that

$$G_0(E) = (E - H_0)^{-1} = \left( E - \frac{p_1^2}{2m_1} - \frac{p_2^2}{2m_2} - \frac{p_3^2}{2m_3} \right)^{-1}$$

so $G_0(E)$ is a function of, and hence commutes with, the momentum operator of particle $\alpha$, $p_\alpha$ (by the functional calculus). Also, it is clear that $p_\alpha$ commutes with $r_\beta$ for $\alpha \neq \beta$ (though not for $\alpha = \beta$ of course) so $p_\alpha$ commutes with $V_\alpha = V_\alpha\left(\left|\mathbf{r}'_\beta - \mathbf{r}'_\gamma\right|\right)$. But, $p_\alpha$ is self-adjoint and has a purely continuous spectrum (section 3.2.2) so by theorem 31, $G_0(E)V_\alpha$ is not a compact operator. Therefore we have no guarantee that the three-body second resolvent equation has a unique solution and hence any solution of this equation obtained numerically should be treated as suspect.

## 5.3 The Faddeev Formulation

When three particles are being considered then, the equations of scattering theory are therefore not entirely satisfactory for calculating the T-matrix or wavefunction. An alternative approach which gives equations with unique solutions is needed. Such an approach was first formulated by *Faddeev* in the early sixties [9], [10] and his brilliant method also yielded the first rigorous proof that the three-body problem was asymptotically complete. Since then, other formulations along similar lines have been proposed, with varying degrees of success. Some of these are discussed in [35] and [16]. Here we shall discuss the basic premises of the Faddeev formulation. However, we will not be able to prove that the equations derived are compact for lack of space. The rigorous proof can be found in [11].

### 5.3.1 Jacobi Coordinates

Recall that in two-body scattering, we worked in the centre of mass coordinate frame (section 4.2.1) which simplified the equations - instead of two variables $\mathbf{r}_1$ and $\mathbf{r}_2$, we only worked in $\mathbf{r}$ (that this assumption does not affect the forms of the operators is discussed in [35], [38]). We have not however, made this assumption yet in the three-body case. We do so now and introduce the Jacobi coordinate systems which have been found to be extremely useful in three-body scattering.

It is customary to use three different coordinate systems, each of two variables, to describe the three-body problem. These shall be denoted by $\mathbf{X}_\alpha = (\mathbf{x}_\alpha, \mathbf{y}_\alpha)$ where $\alpha = 1,2,3$. The origin is the centre of mass of the system and we define our Jacobi coordinates (following [15]) in terms of the particle positions by:

$$\mathbf{x}_\alpha = \sqrt{\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma}}\left(\mathbf{r}_\beta - \mathbf{r}_\gamma\right) \qquad ; \qquad \mathbf{y}_\alpha = \sqrt{\frac{2m_\alpha\left(m_\beta + m_\gamma\right)}{m_\alpha + m_\beta + m_\gamma}}\left(\frac{m_\beta \mathbf{r}_\beta + m_\gamma \mathbf{r}_\gamma}{m_\beta + m_\gamma} - \mathbf{r}_\alpha\right)$$

where $\alpha, \beta$ and $\gamma$ are distinct and refer to the three particles with respective masses $m_\alpha, m_\beta$ and $m_\gamma$. This defines one coordinate system for each particle. In each case (apart from normalising constants), $\mathbf{x}_\alpha$ represents the relative vector between the other two particles and $\mathbf{y}_\alpha$ represents the vector from the particle to the centre of mass of the other two. The three Jacobi coordinates for the momentum $\mathbf{P}_\alpha = (\mathbf{p}_\alpha, \mathbf{q}_\alpha)$ will be defined [11] by:

$$\mathbf{p}_\alpha = \frac{m_\gamma \mathbf{k}_\beta - m_\beta \mathbf{k}_\gamma}{\sqrt{2m_\beta m_\gamma\left(m_\beta + m_\gamma\right)}} \qquad ; \qquad \mathbf{q}_\alpha = \frac{m_\alpha\left[\mathbf{k}_\beta + \mathbf{k}_\gamma\right] - \left[m_\beta + m_\gamma\right]\mathbf{k}_\alpha}{\sqrt{2m_\alpha\left(m_\beta + m_\gamma\right)\left(m_\alpha + m_\beta + m_\gamma\right)}}.$$

Again, $\mathbf{p}_\alpha$ essentially represents the relative momentum between the other two particles whilst $\mathbf{q}_\alpha$ represents the momentum of these particles relative to particle $\alpha$. Of course, it should be clear that each pair of coordinates may be expressed as a linear combination of any other pair of coordinates.

These coordinates, though somewhat complicated, are useful in three-body scattering because they simplify the potential energy operator:

$$V(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = V_1(x_1) + V_2(x_2) + V_3(x_3)$$

where $x_\alpha = |\mathbf{x}_\alpha|$. The normalising constants are chosen so that the kinetic energy operator is:

$$H_0 \supseteq -\nabla^2_{\mathbf{x}_1} - \nabla^2_{\mathbf{y}_1} = -\nabla^2_{\mathbf{x}_2} - \nabla^2_{\mathbf{y}_2} = -\nabla^2_{\mathbf{x}_3} - \nabla^2_{\mathbf{y}_3}$$

in the coordinate representation, and multiplication by the function:

$$H_0(P) = p_1^2 + q_1^2 = p_2^2 + q_2^2 = p_3^2 + q_3^2$$

in the momentum representation.

### 5.3.2 Faddeev Equations for the $\tau$-Operators

Recall that the $\tau$-operators satisfied equation 4.27

$$\tau(E) = V + VG_0(E)\tau(E) = V_1 + V_2 + V_3 + (V_1 + V_2 + V_3)G_0(E)\tau(E).$$

The operator $VG_0$ is not compact in the three-body case so this is not a suitable equation to begin calculations with. The problem is essentially that each term in the potential is only dependent on one variable (in Jacobi coordinates). Such terms are known in the physical literature as *disconnected terms* because in such a term, one of the particles does not interact - it is not 'connected' with the other two. If we were to iterate the equation for the $\tau$-operators however, we get

$$\begin{aligned}\tau(E) &= V_1 + V_2 + V_3 + (V_1 + V_2 + V_3)G_0(E)(V_1 + V_2 + V_3) + \\ &\quad + (V_1 + V_2 + V_3)G_0(E)(V_1 + V_2 + V_3)G_0(E)(V_1 + V_2 + V_3) + \ldots\end{aligned}$$

This equation still contains terms like $V_\alpha G_0(E)V_\alpha$ which are disconnected, but also contains terms of the form of $V_\alpha G_0(E)V_\beta$ $(\beta \neq \alpha)$ which are connected and thus stand a "better chance" of being compact. The key to the Faddeev formulation is to separate the connected and disconnected terms in some way.

Following [11], we decompose $\tau(E)$ into nine operators defined by

$$T_{\alpha\beta}(E) = \delta_{\alpha\beta}V_\alpha + V_\alpha G(E)V_\beta \qquad ; \qquad \alpha,\beta = 1,2,3 \tag{5.10}$$

where $\delta_{\alpha\beta} = 1$ if $\alpha = \beta$ and $\delta_{\alpha\beta} = 0$ otherwise. We can treat these operators as analogues of channel $\tau$-operators as they correspond to processes in which the system is initially in channel $\beta$ and ends up in channel $\alpha$.

These operators do in fact constitute a decomposition as claimed because

$$\begin{aligned}\sum_{\alpha,\beta=1}^{3} T_{\alpha\beta}(E) &= \sum_{\alpha,\beta=1}^{3}\left[\delta_{\alpha\beta}V_\alpha + V_\alpha G(E)V_\beta\right] \\ &= \sum_{\alpha=1}^{3} V_\alpha + \sum_{\alpha=1}^{3} V_\alpha G(E)\sum_{\beta=1}^{3} V_\beta = V + VG(E)V = \tau(E).\end{aligned}$$

Notice that this decomposition partially separates the connected and disconnected terms. All of the disconnected terms are found in the $T_{\alpha\alpha}$-operators (with some connected terms) whereas the terms of the $T_{\alpha\beta}$-operators $(\alpha \neq \beta)$ are all connected.

Using the second resolvent identity on equation 5.10 gives

$$\begin{aligned}T_{\alpha\beta}(E) &= \delta_{\alpha\beta}V_\alpha + V_\alpha[G_0(E) + G_0(E)VG(E)]V_\beta \\ &= \delta_{\alpha\beta}V_\alpha + V_\alpha G_0(E)\left[V_\beta + VG(E)V_\beta\right] \\ &= \delta_{\alpha\beta}V_\alpha + V_\alpha G_0(E)\sum_{\gamma=1}^{3}\left[\delta_{\gamma\beta}V_\beta + V_\gamma G(E)V_\beta\right] \\ &= \delta_{\alpha\beta}V_\alpha + V_\alpha G_0(E)\sum_{\gamma=1}^{3} T_{\gamma\beta}(E)\end{aligned}$$

so these operators satisfy a set of three coupled equations in $\alpha$, for each $\beta$. The operator $V_\alpha G_0(E)$ is not compact so this system is still unsatisfactory. However, this system of equations can be rearranged to give

$$[I - V_\alpha G_0(E)]\, T_{\alpha\beta}(E) = \delta_{\alpha\beta} V_\alpha + V_\alpha G_0(E) \sum_{\gamma \neq \alpha} T_{\gamma\beta}(E). \tag{5.11}$$

Now comes the sneaky part. We proceed to use the two-body problem to solve the three-body problem. We define a two-body $\tau$-operator for each channel, denoting them by $\tau_\alpha(E)$, which acts as if particle $\alpha$ were not present. That is, it acts as if the other two particles constituted a two-body scattering problem by themselves. Recalling that in the Jacobi coordinates for particle $\alpha$, $\mathbf{p}_\alpha$ represents the relative momentum of the other two particles (that is, their momentum if they were treated as a system of their own) whereas $\mathbf{q}_\alpha$ represents the momentum of this "two-body system" relative to particle $\alpha$, we define:

$$\widehat{[\tau_\alpha(E) f]}(\mathbf{p}_\alpha, \mathbf{q}_\alpha) = \int_{\mathbb{R}^3} \tau_\alpha\left(\mathbf{p}_\alpha, \mathbf{p}'_\alpha; E - q_\alpha^2\right) \widehat{f}\left(\mathbf{p}'_\alpha, \mathbf{q}_\alpha\right) d\mathbf{p}'_\alpha$$

where $\tau_\alpha(\mathbf{p}_\alpha, \mathbf{p}'_\alpha; E)$ is the *unique* solution of the two-body off-shell T-matrix equation (4.28):

$$\tau_\alpha\left(\mathbf{p}_\alpha, \mathbf{p}'_\alpha; E\right) = \widehat{V_\alpha}\left(\mathbf{p}_\alpha - \mathbf{p}'_\alpha\right) + \int_{\mathbb{R}^3} \frac{\widehat{V_\alpha}(\mathbf{p}_\alpha - \mathbf{p}''_\alpha)}{E - p''^2_\alpha} \tau_\alpha\left(\mathbf{p}''_\alpha, \mathbf{p}'_\alpha; E\right) d\mathbf{p}''_\alpha.$$

We reduce the energy in the kernel of the defining equation by $q_\alpha^2$ because this is exactly how much kinetic energy we would be neglecting if we ignored particle $\alpha$ and considered the other two particles as a two-body system. It also follows from this reduction that

$$\tau_\alpha\left(\mathbf{p}_\alpha, \mathbf{p}'_\alpha; E - q_\alpha^2\right) = \widehat{V_\alpha}\left(\mathbf{p}_\alpha - \mathbf{p}'_\alpha\right) + \int_{\mathbb{R}^3} \frac{\widehat{V_\alpha}(\mathbf{p}_\alpha - \mathbf{p}''_\alpha)}{E - q_\alpha^2 - p''^2_\alpha} \tau_\alpha\left(\mathbf{p}''_\alpha, \mathbf{p}'_\alpha; E - q_\alpha^2\right) d\mathbf{p}''_\alpha$$

and hence that the $\tau_\alpha$-operators satisfy

$$\tau_\alpha(E) = V_\alpha + V_\alpha G_0(E)\, \tau_\alpha(E) = V_\alpha + \tau_\alpha(E)\, G_0(E) V_\alpha. \tag{5.12}$$

We could not have used *this* relationship to uniquely define the $\tau_\alpha$-operators because the operator $V_\alpha G_0(E)$ is not compact. Notice also that this equation shows that the $\tau_\alpha$-operators contain exactly the disconnected terms of the decomposition of the $\tau$-operator.

These operators are useful because

$$\begin{aligned}
&[I + \tau_\alpha(E) G_0(E)]\,[I - V_\alpha G_0(E)] \\
&\qquad = I - V_\alpha G_0(E) + \tau_\alpha(E) G_0(E) - \tau_\alpha(E) G_0(E) V_\alpha G_0(E) \\
&\qquad\qquad = I + \tau_\alpha(E) G_0(E) - [V_\alpha + \tau_\alpha(E) G_0(E) V_\alpha]\, G_0(E) = I
\end{aligned}$$

so by applying $I + \tau_\alpha(E) G_0(E)$ to equation 5.11, we get

$$T_{\alpha\beta}(E) = \delta_{\alpha\beta}\,[V_\alpha + \tau_\alpha(E) G_0(E) V_\alpha] + [V_\alpha + \tau_\alpha(E) G_0(E) V_\alpha]\, G_0(E) \sum_{\gamma \neq \alpha} T_{\gamma\beta}(E)$$

$$\Rightarrow \quad T_{\alpha\beta}(E) = \delta_{\alpha\beta}\, \tau_\alpha(E) + \tau_\alpha(E) G_0(E) \sum_{\gamma \neq \alpha} T_{\gamma\beta}(E). \tag{5.13}$$

These are the *Faddeev equations* for the $T_{\alpha\beta}$-operators and are a set of three coupled equations in $\alpha$, for each $\beta$. In matrix form, these become (for $\beta = 1$)

$$\begin{pmatrix} T_{11} \\ T_{21} \\ T_{31} \end{pmatrix} = \begin{pmatrix} \tau_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & \tau_1 G_0 & \tau_1 G_0 \\ \tau_2 G_0 & 0 & \tau_2 G_0 \\ \tau_3 G_0 & \tau_3 G_0 & 0 \end{pmatrix} \begin{pmatrix} T_{11} \\ T_{21} \\ T_{31} \end{pmatrix}$$

(for $\beta \neq 1$, the first term on the right hand side is $\tau_\beta$ in the $\beta$-th entry and 0 elsewhere). Since we generally begin a scattering experiment in a definite channel $\beta$ rather than a superposition of channels, we will lose no generality by defining new operators

$$T^{(\alpha)} = \sum_{\beta=1}^{3} T_{\alpha\beta}$$

which obey the $T^{(\alpha)}$-operator Faddeev equations

$$T^{(\alpha)} = \tau_\alpha(E) + \tau_\alpha(E) G_0(E) \sum_{\gamma\neq\alpha} T^{(\gamma)} \tag{5.14}$$

derived by summing the $T_{\alpha\beta}$-operator equations over $\beta$. The matrix form of these equations is

$$\begin{pmatrix} T^{(1)} \\ T^{(2)} \\ T^{(3)} \end{pmatrix} = \begin{pmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \end{pmatrix} + \begin{pmatrix} 0 & \tau_1 G_0 & \tau_1 G_0 \\ \tau_2 G_0 & 0 & \tau_2 G_0 \\ \tau_3 G_0 & \tau_3 G_0 & 0 \end{pmatrix} \begin{pmatrix} T^{(1)} \\ T^{(2)} \\ T^{(3)} \end{pmatrix}$$

so the only difference is in the first term. These $T^{(\alpha)}$-equations were first derived by Faddeev in [9].

Although the 'matrix kernel' of this set of equations is still disconnected, its square (corresponding to an iteration of this equation) and higher powers have only connected entries so the only disconnected parts of the iterated equations are in the first two terms of the iteration. Faddeev was able to prove [11] that these equations did have a unique solution by constructing an appropriate *Banach space* in which Fredholm theory could be applied to his formulation, under the following restrictions on the two-body potentials:

$$\begin{aligned} \left|\widehat{V_\alpha}(p_\alpha)\right| &\leqslant C(1+p_\alpha)^{-1-\varepsilon} \qquad (C>0, \varepsilon>0) \\ \left|\widehat{V_\alpha}(p_\alpha+h) - \widehat{V_\alpha}(p_\alpha)\right| &\leqslant C(1+p_\alpha)^{-1-\varepsilon}|h|^\mu \qquad (\mu>0). \end{aligned}$$

This of course has been extended and modified since then to cover other cases (especially the Coulomb potential) and generalised to $N$-body scattering problems [12].

### 5.3.3 Faddeev Equations for the Full Green's Operator

The Faddeev equations we have derived are most easily examined in the momentum representation. However, as is noted in [15], it is now possible to use the Faddeev equations in momentum space to study the continuity and asymptotic behaviour of the wavefunction in coordinate space. That is, the boundary conditions appropriate to the three-body Schrödinger equation can now be derived. This is of great importance because solving the Faddeev equations in momentum space often involves evaluating integrals in which the kernel has singularities. It turns out however, that the boundary conditions for the Schrödinger equation are much too complicated to be of any practical use. Instead the wavefunction may be decomposed into a sum of functions, each written in terms of a particular Jacobi coordinate system, to which somewhat more tractable boundary conditions can be applied. We will not give the boundary conditions here, they can be found in [12] or [15].

To derive equations for the components of the wavefunction, we first show that the full Green's operator can be decomposed into component operators, as we did for the $\tau$-operator in the previous section. Define the *component Green's operators* in terms of the Faddeev $T^{(\alpha)}$-operators by

$$G^{(\alpha)}(E) = G_0(E) T^{(\alpha)}(E) G_0(E).$$

We therefore have

$$\begin{aligned} G(E) &= G_0(E) + G(E)VG_0(E) = G_0(E) + G_0(E)\tau(E)G_0(E) \\ &= G_0(E) + G_0(E)\sum_{\alpha=1}^{3} T^{(\alpha)}(E)G_0(E) = G_0(E) + \sum_{\alpha=1}^{3} G^{(\alpha)}(E) \end{aligned} \tag{5.15}$$

as required. Furthermore, multiplying the Faddeev equations for the $T^{(\alpha)}$-operators by $G_0(E)$ from the left and the right gives

$$G^{(\alpha)}(E) = G_0(E)\,\tau_\alpha(E)\,G_0(E) + G_0(E)\,\tau_\alpha(E)\sum_{\gamma\neq\alpha} G^{(\gamma)}(E)$$

$$\Rightarrow \quad G^{(\alpha)}(E) = [G_\alpha(E) - G_0(E)] + G_\alpha(E)\,V_\alpha \sum_{\gamma\neq\alpha} G^{(\gamma)}(E), \tag{5.16}$$

where we have used equation 5.8 and the easily verified relations

$$V_\alpha G_\alpha(E) = \tau_\alpha(E)\,G_0(E) \qquad \text{and} \qquad G_\alpha(E)\,V_\alpha = G_0(E)\,\tau_\alpha(E). \tag{5.17}$$

This system of equations for the components of the full Green's operator is sometimes called the Faddeev equations for the $G^{(\alpha)}$-operators.

### 5.3.4 The Coordinate Representation

These $G^{(\alpha)}$-operator equations will provide the means to derive a set of equations for the wavefunction of the system. To do this however, we must introduce the asymptotic wavefunctions relevant to the three-body problem. For the channel in which the three particles are free, the asymptotic wavefunction is the free plane wave

$$\phi_{\mathbf{P}}(\mathbf{X}) = \frac{1}{(2\pi)^3} e^{i\mathbf{P}\cdot\mathbf{X}}$$

and since $\mathbf{P}_1\cdot\mathbf{X}_1 = \mathbf{P}_2\cdot\mathbf{X}_2 = \mathbf{P}_3\cdot\mathbf{X}_3$, it doesn't matter which Jacobi coordinate system we work in. Similarly, if the system is initially in the channel in which particle $\beta$ is free and the other two particles form a bound state, then we have the asymptotic wavefunctions

$$\phi_{n,\mathbf{q}_\beta}(\mathbf{x}_\beta, \mathbf{y}_\beta) = \frac{1}{(2\pi)^3}\chi_\beta^{(n)}(\mathbf{x}_\beta)\, e^{i\mathbf{q}_\beta\cdot\mathbf{y}_\beta}$$

where $\chi_\beta^{(n)}(\mathbf{x}_\beta)$ is the wavefunction corresponding to the bound state formed and $n$ is a quantum number identifying which bound state is formed (in the event that there are excited states) [15]. We will in the following be interested in scattering processes with these initial states, so we will therefore assume these asymptotic wavefunctions.

Consider the decomposition of the full Green's operator (equation 5.15):

$$G(E) = G_0(E) + \sum_{\alpha=1}^{3} G^{(\alpha)}(E).$$

Of course, we assume that the $G^{(\alpha)}$-operators are integral operators with kernel functions $G^{(\alpha)}(\mathbf{X}_\alpha, \mathbf{X}'_\alpha; E)$ in their $\alpha$-Jacobi coordinate system. We note that because the form of $G_0(E)$ in the momentum representation is independent of the Jacobi coordinates used, this must also be true for its kernel in the coordinate representation. However, the corresponding statements are by no means true for the $G^{(\alpha)}$-operators. The functional forms of their kernels are dependent upon which Jacobi coordinates are used.

Expanding this equation in arbitrary Jacobi coordinates (labelled by $\beta$) gives for $f \in S(\mathbb{R}^6)$:

$$\int_{\mathbb{R}^6} G\left(\mathbf{X}_\beta, \mathbf{X}'_\beta; E\right) f\left(\mathbf{X}'_\beta\right) d\mathbf{X}'_\beta = \int_{\mathbb{R}^6} G_0\left(\mathbf{X}_\beta, \mathbf{X}'_\beta; E\right) f\left(\mathbf{X}'_\beta\right) d\mathbf{X}'_\beta + \sum_{\alpha=1}^{3}\left[G^{(\alpha)}(E)\, f\right](\mathbf{X}_\beta).$$

Now, since the different Jacobi coordinates are all linearly dependent, $\mathbf{X}_\beta$ can be written as a function of $\mathbf{X}_\alpha$, $\mathbf{X}_\beta(\mathbf{X}_\alpha)$ and vice versa. Therefore, the last term of the previous equation

may be rewritten as

$$\begin{aligned}\sum_{\alpha=1}^{3}\left[G^{(\alpha)}(E)\,f\right](\mathbf{X}_\beta) &= \sum_{\alpha=1}^{3}\left[G^{(\alpha)}(E)\,f\right]\left[\mathbf{X}_\beta(\mathbf{X}_\alpha)\right] \\ &= \sum_{\alpha=1}^{3}\int_{\mathbb{R}^6} G^{(\alpha)}\left(\mathbf{X}_\alpha,\mathbf{X}'_\alpha;E\right) f\left(\mathbf{X}_\beta\left(\mathbf{X}'_\alpha\right)\right) d\mathbf{X}'_\alpha.\end{aligned}$$

It can be readily verified (see [15]) that the Jacobian of the coordinate change from $\mathbf{X}_\alpha$ to $\mathbf{X}_\beta$ is 1 (as one would expect) so

$$\sum_{\alpha=1}^{3}\left[G^{(\alpha)}(E)\,f\right](\mathbf{X}_\beta) = \sum_{\alpha=1}^{3}\int_{\mathbb{R}^6} G^{(\alpha)}\left(\mathbf{X}_\alpha(\mathbf{X}_\beta),\mathbf{X}_\alpha\left(\mathbf{X}'_\beta\right);E\right) f\left(\mathbf{X}'_\beta\right) d\mathbf{X}'_\beta.$$

Therefore, if we extract the kernel of the original equation, we get

$$G\left(\mathbf{X}_\beta,\mathbf{X}'_\beta;E\right) = G_0\left(\mathbf{X}_\beta,\mathbf{X}'_\beta;E\right) + \sum_{\alpha=1}^{3} G^{(\alpha)}\left(\mathbf{X}_\alpha,\mathbf{X}'_\alpha;E\right). \tag{5.18}$$

To introduce the wavefunctions into these equations, we recall equation 4.9:

$$\Omega_\pm = \mathrm{s}-\lim_{\varepsilon\to 0^+} \pm i\varepsilon\left[\int_{\mathbb{R}^3} G(\lambda\pm i\varepsilon)\,dE_\lambda^{H_0}\right].$$

Performing an eigenfunction expansion on this equation yields the kernel equation:

$$\phi^+_{n,\mathbf{q}_\beta}(\mathbf{X}_\beta) = \lim_{\varepsilon\to 0^+} i\varepsilon\int_{\mathbb{R}^6} G\left(\mathbf{X}_\beta,\mathbf{X}'_\beta;E+i\varepsilon\right)\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right) d\mathbf{X}'_\beta \tag{5.19}$$

where $E$ is the energy of the system, $\phi_{n,\mathbf{q}_\beta}(\mathbf{X}_\beta)$ is the incoming asymptotic wavefunction of the system, and $\phi^+_{n,\mathbf{q}_\beta}(\mathbf{X}_\beta)$ is the actual wavefunction. Analogously, we *define* the functions ($\alpha = 1,2,3$):

$$\phi_n^{(\alpha)}(\mathbf{X}_\alpha) = \lim_{\varepsilon\to 0^+} i\varepsilon\int_{\mathbb{R}^6} G^{(\alpha)}\left(\mathbf{X}_\alpha,\mathbf{X}'_\alpha;E+i\varepsilon\right)\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}_\beta\left(\mathbf{X}'_\alpha\right)\right) d\mathbf{X}'_\alpha. \tag{5.20}$$

Multiplying our kernel equation by $i\varepsilon\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right)$, integrating over all particle positions (changing the variables of integration where necessary) and then taking the limit as $\varepsilon\to 0^+$, we finally get the result that the total wavefunction may be expressed by

$$\phi^+_{n,\mathbf{q}_\beta}(\mathbf{X}) = \sum_{\alpha=1}^{3}\phi_n^{(\alpha)}(\mathbf{X}_\alpha). \tag{5.21}$$

(For simplicity, we've dropped the $\beta$ subscripts so our arbitrary Jacobi coordinates are denoted by $\mathbf{X}$.) That is, the total wavefunction can be decomposed into component wavefunctions which are nicely expressed in different Jacobi coordinates. Although the kernel equation contained the additional term $G_0(\mathbf{X},\mathbf{X}';E)$, there is nothing in our wavefunction decomposition corresponding to this term. This is due to the relation

$$\lim_{\varepsilon\to 0^+} i\varepsilon\int_{\mathbb{R}^6} G_0\left(\mathbf{X}_\beta,\mathbf{X}'_\beta;E+i\varepsilon\right)\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right) d\mathbf{X}'_\beta = 0, \tag{5.22}$$

the proof of which we shall defer to an appendix (section 5.3.5) to avoid disrupting continuity.

We now apply the operator $(E-H_\alpha)$ to the $G^{(\alpha)}$-operator Faddeev equations giving

$$\begin{aligned}(E-H_\alpha)G^{(\alpha)}(E) &= (E-H_\alpha)\left[G_\alpha(E)-G_0(E)\right] + (E-H_\alpha)G_\alpha(E)V_\alpha\sum_{\gamma\neq\alpha}G^{(\gamma)}(E) \\ &= \left[I-(E-H_0-V_\alpha)G_0(E)\right] + V_\alpha\sum_{\gamma\neq\alpha}G^{(\gamma)}(E) \\ &= V_\alpha\left[G_0(E)+\sum_{\gamma\neq\alpha}G^{(\gamma)}(E)\right].\end{aligned}$$

Making the familiar eigenfunction expansion of this equation then gives

$$\left[E+\nabla_{\mathbf{X}}^2-V_\alpha\left(x_\alpha\right)\right]\phi_n^{(\alpha)}\left(\mathbf{X}_\alpha\right)=V_\alpha\left(x_\alpha\right)\sum_{\gamma\neq\alpha}\phi_n^{(\gamma)}\left(\mathbf{X}_\gamma\right) \tag{5.23}$$

where the $G_0$-term again vanishes (section 5.3.5). These are the *differential Faddeev equations* and are a coupled set of equations which are satisfied by the components of the wavefunction, and may be solved subject to the appropriate boundary conditions (see [15]).

### 5.3.5 Appendix

We now prove that equation 5.22

$$\lim_{\varepsilon\to 0^+} i\varepsilon\int_{\mathbb{R}^6} G_0\left(\mathbf{X}_\beta,\mathbf{X}'_\beta;E+i\varepsilon\right)\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right)d\mathbf{X}'_\beta=0$$

holds, as claimed above. We begin by noting that

$$\begin{aligned}
\left[G_0\left(z\right)f\right]\left(\mathbf{X}\right) &= \frac{1}{\left(2\pi\right)^3}\int_{\mathbb{R}^6}\left[G_0\left(z\right)f\right]\hat{}\left(\mathbf{P}\right)e^{i\mathbf{P}\cdot\mathbf{X}}d\mathbf{P}=\frac{1}{\left(2\pi\right)^3}\int_{\mathbb{R}^6}\frac{\widehat{f}\left(\mathbf{P}\right)}{z-P^2}e^{i\mathbf{P}\cdot\mathbf{X}}d\mathbf{P}\\
&= \frac{1}{\left(2\pi\right)^6}\int_{\mathbb{R}^6}\frac{e^{i\mathbf{P}\cdot\mathbf{X}}}{z-P^2}\left[\int_{\mathbb{R}^6}f\left(\mathbf{X}'\right)e^{-i\mathbf{P}\cdot\mathbf{X}'}d\mathbf{X}'\right]d\mathbf{P}\\
&= \frac{1}{\left(2\pi\right)^6}\int_{\mathbb{R}^6}\left[\int_{\mathbb{R}^6}\frac{e^{i\mathbf{P}\cdot\left(\mathbf{X}-\mathbf{X}'\right)}}{z-P^2}d\mathbf{P}\right]f\left(\mathbf{X}'\right)d\mathbf{X}'\\
&\Rightarrow\quad G_0\left(\mathbf{X},\mathbf{X}';z\right)=\frac{1}{\left(2\pi\right)^6}\int_{\mathbb{R}^6}\frac{e^{i\mathbf{P}\cdot\left(\mathbf{X}-\mathbf{X}'\right)}}{z-P^2}d\mathbf{P}.
\end{aligned}$$

It follows then that

$$\begin{aligned}
&\int_{\mathbb{R}^6}G_0\left(\mathbf{X}_\beta,\mathbf{X}'_\beta;E+i\varepsilon\right)\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right)d\mathbf{X}'_\beta\\
&= \frac{1}{\left(2\pi\right)^6}\int_{\mathbb{R}^6}\left[\int_{\mathbb{R}^6}\frac{e^{i\mathbf{P}'_\beta\cdot\left(\mathbf{X}_\beta-\mathbf{X}'_\beta\right)}}{z-P'^2_\beta}d\mathbf{P}'_\beta\right]\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right)d\mathbf{X}'_\beta\\
&= \frac{1}{\left(2\pi\right)^9}\int_{\mathbb{R}^{12}}\frac{e^{i\mathbf{p}'_\beta\cdot\left(\mathbf{x}_\beta-\mathbf{x}'_\beta\right)}e^{i\mathbf{q}'_\beta\cdot\left(\mathbf{y}_\beta-\mathbf{y}'_\beta\right)}}{z-p'^2_\beta-q'^2_\beta}\chi_\beta^{(n)}\left(\mathbf{x}'_\beta\right)e^{i\mathbf{q}_\beta\cdot\mathbf{y}'_\beta}d\mathbf{p}'_\beta d\mathbf{q}'_\beta d\mathbf{x}'_\beta d\mathbf{y}'_\beta\\
&= \frac{1}{\left(2\pi\right)^9}\int_{\mathbb{R}^9}\frac{e^{i\mathbf{p}'_\beta\cdot\left(\mathbf{x}_\beta-\mathbf{x}'_\beta\right)}\chi_\beta^{(n)}\left(\mathbf{x}'_\beta\right)e^{i\mathbf{q}'_\beta\cdot\mathbf{y}_\beta}}{z-p'^2_\beta-q'^2_\beta}\left[\int_{\mathbb{R}^3}e^{i\left(\mathbf{q}_\beta-\mathbf{q}'_\beta\right)\cdot\mathbf{y}'_\beta}d\mathbf{y}'_\beta\right]d\mathbf{p}'_\beta d\mathbf{q}'_\beta d\mathbf{x}'_\beta\\
&= \frac{1}{\left(2\pi\right)^{15/2}}\int_{\mathbb{R}^6}e^{i\mathbf{p}'_\beta\cdot\left(\mathbf{x}_\beta-\mathbf{x}'_\beta\right)}\chi_\beta^{(n)}\left(\mathbf{x}'_\beta\right)\left[\int_{\mathbb{R}^3}\frac{e^{i\mathbf{q}'_\beta\cdot\mathbf{y}_\beta}}{z-p'^2_\beta-q'^2_\beta}\delta\left(\mathbf{q}_\beta-\mathbf{q}'_\beta\right)d\mathbf{q}'_\beta\right]d\mathbf{p}'_\beta d\mathbf{x}'_\beta\\
&= \frac{e^{i\mathbf{q}_\beta\cdot\mathbf{y}_\beta}}{\left(2\pi\right)^{15/2}}\int_{\mathbb{R}^3}\left[\int_{\mathbb{R}^3}\frac{e^{i\mathbf{p}'_\beta\cdot\left(\mathbf{x}_\beta-\mathbf{x}'_\beta\right)}}{z-p'^2_\beta-q_\beta^2}d\mathbf{p}'_\beta\right]\chi_\beta^{(n)}\left(\mathbf{x}'_\beta\right)d\mathbf{x}'_\beta
\end{aligned}$$

where we have used equation 1.5. Comparing the integral over $\mathbf{p}'_\beta$ with the form of the free Green's function we derived earlier, we see that this is just a two-body free Green's function. Therefore,

$$\int_{\mathbb{R}^6}G_0\left(\mathbf{X}_\beta,\mathbf{X}'_\beta;z\right)\phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right)d\mathbf{X}'_\beta=\frac{e^{i\mathbf{q}_\beta\cdot\mathbf{y}_\beta}}{\left(2\pi\right)^{9/2}}\int_{\mathbb{R}^3}\frac{-e^{i\sqrt{z-q_\beta^2}\left|\mathbf{x}_\beta-\mathbf{x}'_\beta\right|}}{4\pi\left|\mathbf{x}_\beta-\mathbf{x}'_\beta\right|}\chi_\beta^{(n)}\left(\mathbf{x}'_\beta\right)d\mathbf{x}'_\beta$$

$$\Rightarrow \left| \int_{\mathbb{R}^6} G_0\left(\mathbf{X}_\beta, \mathbf{X}'_\beta; z\right) \phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right) d\mathbf{X}'_\beta \right| \leqslant \frac{1}{(2\pi)^{9/2}} \int_{\mathbb{R}^3} \frac{\left|\chi_\beta^{(n)}\left(\mathbf{x}'_\beta\right)\right|}{4\pi \left|\mathbf{x}_\beta - \mathbf{x}'_\beta\right|} d\mathbf{x}'_\beta .$$

Given that $\chi_\beta^{(n)}\left(\mathbf{x}'_\beta\right)$ is a bound state wavefunction and therefore decreases rapidly [32], it is easily seen that this integral converges for any $\mathbf{x}_\beta$, and is independent of $z$. Letting $z = E + i\varepsilon$ then, multiplying by $i\varepsilon$ and taking the limit as $\varepsilon \to 0^+$ gives

$$\lim_{\varepsilon \to 0^+} i\varepsilon \int_{\mathbb{R}^6} G_0\left(\mathbf{X}_\beta, \mathbf{X}'_\beta; E + i\varepsilon\right) \phi_{n,\mathbf{q}_\beta}\left(\mathbf{X}'_\beta\right) d\mathbf{X}'_\beta = 0$$

as required.

# Chapter 6

# A Separable Three-Body Problem

*"I don't even want you to begin to start explainin' that. You're probably goin' to go on about the universe bein' a rubber sheet with weights on it again, right? And the word* 'quantum' *is hurryin' towards your lips again.*"

Archchancellor Mustrum Ridcully

## 6.1 Non-Local Interactions

### 6.1.1 The Separable Approximation

So far in discussing potentials, we have restricted attention to potentials of the form $V = V(r)$ where $r$ is the distance between the particles. This represents an interaction where the force felt by one of the particles essentially emanates from the position of the other particle and is known in the physical literature as a *local potential*. That is, the interaction derives from point sources. However, we can also envisage scenarios in which it would be useful to model an interaction in other ways. For instance in nucleon scattering, we could let the interaction derive from a small non-zero volume of space, the nucleus, so as to better account for internal structure. In any case, these more general interactions correspond to potential energy operators which are not of the form $V(r)$. These are known as *non-local interactions*.

As an important example of a non-local interaction, we shall discuss the *separable potentials*. These are defined in operator form for any $f$ in the Hilbert space by

$$Vf = \lambda \langle a, f \rangle a \tag{6.1}$$

where $a$ is a fixed vector from the Hilbert space (usually chosen such that $\|a\| = 1$) and $\lambda \in \mathbb{R}$ is a constant representing the strength of the interaction (negative for attractive potentials, positive for repulsive potentials). If we recast this equation in $L^2(\mathbb{R}^n)$, we find that

$$(Vf)(\mathbf{r}) = \lambda \int_{\mathbb{R}^n} \overline{a(\mathbf{r}')} f(\mathbf{r}') \, d\mathbf{r}' a(\mathbf{r}) = \int_{\mathbb{R}^n} \lambda a(\mathbf{r}) \overline{a(\mathbf{r}')} f(\mathbf{r}') \, d\mathbf{r}' \tag{6.2}$$

so $V$ becomes an integral operator with a separable kernel $\lambda a(\mathbf{r}) \overline{a(\mathbf{r}')}$. The function $a(\mathbf{r})$ is called the *form factor* for the interaction. Potentials of this kind have been found to give reasonable results in some areas of nuclear physics [45].

Now, $V$ is not a multiplication operator but is bounded since

$$\|Vf\| = |\lambda \langle a, f \rangle| \, \|a\| \leqslant |\lambda| \, \|a\|^2 \, \|f\| \quad \Rightarrow \quad \|V\| \leqslant |\lambda| \, \|a\|^2 .$$

Furthermore, $V$ is symmetric:

$$\langle Vf, g \rangle = \langle \lambda \langle a, f \rangle a, g \rangle = \lambda \overline{\langle a, f \rangle} \langle a, g \rangle = \lambda \langle f, a \rangle \langle a, g \rangle = \langle f, \lambda \langle a, g \rangle a \rangle = \langle f, Vg \rangle$$

hence self-adjoint. In fact, if $\lambda = 1$, $V$ is just the projection operator onto the subspace spanned by $\{a\}$. Since $V$ is bounded, it has $H_0$-bound 0 (section 3.3.2) and so by theorem 26, $H = H_0 + V$ is a bona-fide self-adjoint operator.

In fact, the separable potentials are known to mathematicians as the *rank one compact operators*. Compactness is established (recalling the definition in section 5.2.1) by noting that for any uniformly bounded sequence $(f_n)$, $(\langle a, f_n\rangle)$ is a uniformly bounded sequence of numbers which must therefore have a convergent subsequence: $\langle a, f_{n_k}\rangle \to \omega$ say, as $k \to \infty$. But then, $(Vf_n)$ has a convergent subsequence $(Vf_{n_k})$ because

$$\lim_{k\to\infty} V f_{n_k} = \lim_{k\to\infty} \langle a, f_{n_k}\rangle a = \omega a$$

so $V$ is compact. Now, while compactness of integral operators is a much desired property in mathematical physics (section 5.2), it can be problematic in the present case due to a well-known result of Weyl and Von-Neumann (see [2]). This states that in a separable Hilbert space, there are self-adjoint compact operators which when added to an operator with a continuous spectrum, result in an operator with only point spectrum. $H_0$ has a continuous spectrum and $V$ is self-adjoint and compact, so it is possible that $H = H_0 + V$ has only point spectrum. Such a Hamiltonian has no place in scattering theory as there are no free states! That this is not the case for the separable potential is proved in [26] who shows that the wave operators exist for these separable potentials and are complete (section 10.4.2, theorem 4.3).

### 6.1.2 The Two-Body Problem with a Separable Potential

There is a definite advantage to considering scattering equations with separable potentials. The advantage is that the equations are far more tractable and in the two-body case, admit analytical solutions. Let us illustrate this by considering this case. Recall the equation for the $\tau$-operator (equation 4.28):

$$\tau\left(\mathbf{k},\mathbf{k}';E\right) = \widehat{V}\left(\mathbf{k}-\mathbf{k}'\right) + \int_{\mathbb{R}^3} \frac{\widehat{V}\left(\mathbf{k}-\mathbf{k}''\right)}{E-k''^2}\tau\left(\mathbf{k}'',\mathbf{k}';E\right)d\mathbf{k}''.$$

Recalling the coordinate representation for a separable potential (equation 6.2), we have that

$$\begin{aligned}\widehat{V}\left(\mathbf{k}-\mathbf{k}'\right) = \int_{\mathbb{R}^3} \overline{\phi_{\mathbf{k}}(\mathbf{r})} V \phi_{\mathbf{k}'}\left(\mathbf{r}'\right) d\mathbf{r} &= \int_{\mathbb{R}^3} \overline{\phi_{\mathbf{k}}(\mathbf{r})}\left[\int_{\mathbb{R}^3} \lambda a(\mathbf{r})\overline{a(\mathbf{r}')}\phi_{\mathbf{k}'}\left(\mathbf{r}'\right)d\mathbf{r}'\right]d\mathbf{r} \\ &= \lambda\left[\int_{\mathbb{R}^3} a(\mathbf{r})\overline{\phi_{\mathbf{k}}(\mathbf{r})}d\mathbf{r}\right]\left[\int_{\mathbb{R}^3}\overline{a(\mathbf{r}')}\phi_{\mathbf{k}'}\left(\mathbf{r}'\right)d\mathbf{r}'\right] = \lambda\widehat{a}(\mathbf{k})\overline{\widehat{a}(\mathbf{k}')}.\end{aligned}$$

Substitution into the $\tau$-operator equation therefore gives

$$\tau\left(\mathbf{k},\mathbf{k}';E\right) = \lambda\widehat{a}(\mathbf{k})\overline{\widehat{a}(\mathbf{k}')} + \int_{\mathbb{R}^3}\frac{\lambda\widehat{a}(\mathbf{k})\overline{\widehat{a}(\mathbf{k}'')}}{E-k''^2}\tau\left(\mathbf{k}'',\mathbf{k}';E\right)d\mathbf{k}'' = \lambda\widehat{a}(\mathbf{k})\,\kappa\left(\mathbf{k}'\right) \tag{6.3}$$

where

$$\kappa\left(\mathbf{k}'\right) = \overline{\widehat{a}(\mathbf{k}')} + \int_{\mathbb{R}^3}\frac{\overline{\widehat{a}(\mathbf{k}'')}}{E-k''^2}\tau\left(\mathbf{k}'',\mathbf{k}';E\right)d\mathbf{k}''. \tag{6.4}$$

Substituting 6.3 into 6.4 then allows us to solve for the off-shell T-matrix:

$$\begin{aligned}\kappa\left(\mathbf{k}'\right) &= \overline{\widehat{a}(\mathbf{k}')} + \int_{\mathbb{R}^3}\frac{\overline{\widehat{a}(\mathbf{k}'')}}{E-k''^2}\lambda\widehat{a}\left(\mathbf{k}''\right)\kappa\left(\mathbf{k}'\right)d\mathbf{k}'' = \overline{\widehat{a}(\mathbf{k}')} + \lambda\,\kappa\left(\mathbf{k}'\right)\int_{\mathbb{R}^3}\frac{|\widehat{a}(\mathbf{k}'')|^2}{E-k''^2}d\mathbf{k}'' \\ \Rightarrow \quad \kappa\left(\mathbf{k}'\right) &= \frac{\overline{\widehat{a}(\mathbf{k}')}}{1-\lambda\int_{\mathbb{R}^3}\frac{|\widehat{a}(\mathbf{k}'')|^2}{E-k''^2}d\mathbf{k}''} \\ \Rightarrow \quad \tau\left(\mathbf{k},\mathbf{k}';E\right) &= \frac{\lambda\widehat{a}(\mathbf{k})\overline{\widehat{a}(\mathbf{k}')}}{1-\lambda\int_{\mathbb{R}^3}\frac{|\widehat{a}(\mathbf{k}'')|^2}{E-k''^2}d\mathbf{k}''}.\end{aligned} \tag{6.5}$$

We note that it may be possible for the denominator of this expression to vanish as $\mathrm{Im}E \to 0^+$, in which case, the T-matrix does not exist. It is not hard to see that a consequence of this is that

$\lim_{\varepsilon\to 0^+} G(\mathbf{r},\mathbf{r}';E+i\varepsilon)$ does not exist and therefore that we are dealing with energies in the point spectrum - bound states. In fact (assuming that $\lambda<0$ so we have an attractive potential), $\left(E-k''^2\right)^{-1}$ decreases from 0 to $-k''^{-2}$ as $E$ increases from $-\infty$ to 0 for any $k''\in\mathbb{R}$. Thus the second term in the denominator must be increasing from 0 to $|\lambda|\int_{\mathbb{R}^3}|\widehat{a}(\mathbf{k}'')|^2/k''^2 d\mathbf{k}''$ so the denominator may only vanish once. Therefore, if there is a bound state corresponding to an attractive separable potential, there is only one. It is easy to see that a repulsive separable potential does not support any bound states, as one would expect.

Let us now consider the particular case of a separable potential with form factor $a(\mathbf{r})=e^{-\Lambda r}/r$ ($\Lambda>0$). We have

$$\widehat{a}(\mathbf{k})=\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\frac{e^{-\Lambda r}}{r}e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}=\sqrt{\frac{2}{\pi}}\frac{1}{\Lambda^2+k^2}. \tag{6.6}$$

To calculate the T-matrix, we need to evaluate the following expression. This is quite messy and is best calculated using a computer algebra package giving

$$\begin{aligned}\lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}\frac{|\widehat{a}(\mathbf{k}'')|^2}{E+i\varepsilon-k''^2}d\mathbf{k}''&=\lim_{\varepsilon\to 0^+}\int_0^\infty\frac{8k''^2dk''}{(E+i\varepsilon-k''^2)(\Lambda^2+k^2)^2}\\&=\frac{-2\pi\left(\Lambda^2+2i\sqrt{E}\Lambda-E\right)}{\Lambda(\Lambda^2+E)^2}=\frac{-2\pi}{\Lambda\left(\Lambda-i\sqrt{E}\right)^2}\end{aligned}$$

where $\sqrt{E}=i\sqrt{-E}$ if $E<0$. Assuming $E>0$, we find that the T-matrix is explicitly given by

$$\begin{aligned}t\left(\mathbf{k},\mathbf{k}'\right)=\lim_{\varepsilon\to 0^+}\tau\left(\mathbf{k},\mathbf{k}';k'^2+i\varepsilon\right)&=\lim_{\varepsilon\to 0^+}\frac{\lambda\widehat{a}(\mathbf{k})\overline{\widehat{a}(\mathbf{k}')}}{1-\lambda\int_{\mathbb{R}^3}\frac{|\widehat{a}(\mathbf{k}'')|^2}{k'^2+i\varepsilon-k''^2}d\mathbf{k}''}\\&=\frac{2\lambda}{\pi(\Lambda^2+k^2)(\Lambda^2+k'^2)\left(1+\frac{2\pi\lambda}{\Lambda(\Lambda-ik')^2}\right)}.\end{aligned}$$

so the differential cross-section is given by

$$\frac{d\sigma}{d\Omega}=\frac{16\pi^2\lambda^2}{(\Lambda^2+k^2)^4\left|1+\frac{2\pi\lambda}{\Lambda(\Lambda-ik)^2}\right|^2}.$$

## 6.2 Angular Momentum

We have so far completely ignored the important angular quantities and their role in quantum mechanics. In fact, one can define an angular momentum operator in three dimensions by $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ as one does in classical mechanics (the $\times$ denotes vector cross-product). This operator and its component operators may be proven self-adjoint [38] and are as important in scattering theory as the position operators are. In fact, one can derive an eigenfunction expansion theory based on these operators which leads to the important theory of partial waves (see [35] for instance). However, it is not this "classical" (or orbital) angular momentum which we wish to discuss here. Rather, we shall need to introduce the concept of intrinsic particle spin and how it may affect a scattering process.

### 6.2.1 Intrinsic Particle Spin

It is an experimentally observed fact that fundamental particles possess an intrinsic angular momentum that is quite different to any orbital angular momentum. The basis for this is the

famous *Stern-Gerlach experiment* and a description of these experiments and their importance in the development of quantum theory can be found in any introductory text on quantum theory (see [31] or [46]). We therefore introduce an intrinsic spin operator $\mathbf{S} = (S_x, S_y, S_z)$, analogous to the orbital angular momentum operator mentioned above, which represents the observable quantity of total intrinsic spin. Particles have been found experimentally to have one of the total spin values: $0, 1/2, 1, 3/2, 2, \ldots$

It is customary to discuss the component of the spin operator in the $z$-direction, $S_z$. Experiment shows that this observable is quantised - if $s$ is the total spin of the particle, $s_z$ may take any of the $2s+1$ values, $-s, -s+1, ..., s-1, s$. That is, for a spin-$1/2$ particle (for instance, an electron or a proton), $s_z$ can be $-1/2$ or $1/2$. We therefore construct a spin Hilbert space, $\mathscr{H}_{spin}$, separate from the usual coordinate Hilbert space, for the particle by defining eigenvectors $f_{s_z}$ which are such that

$$S_z f_{s_z} = s_z f_{s_z}$$

for all allowed values of $s_z$, and letting $\mathscr{H}_{spin}$ be the space of all linear combinations of the $f_{s_z}$ with an appropriate inner-product. This is therefore a $2s+1$-dimensional Hilbert space. A convenient choice for this space is the space $\ell^2(2s+1)$ of sequences of length $2s+1$.

To account for a particle with spin $s$ then, we introduce the combined Hilbert space

$$\mathscr{H}_{total} = \mathscr{H}_{coord} \otimes \mathscr{H}_{spin} \cong L^2\left(\mathbb{R}^3\right) \otimes \ell^2(2s+1)$$

which is the tensor product of the usual coordinate Hilbert space and the spin space. In the case we have been examining with three particles (each of which may now have spin), the appropriate Hilbert space is

$$L^2\left(\mathbb{R}^6\right) \otimes \ell^2(2s+1) \otimes \ell^2(2s+1) \otimes \ell^2(2s+1)$$

after factoring out the centre of mass motion which reduces the number of coordinates needed from 9 to 6.

### 6.2.2 Identical Particles and Symmetrisation

We have introduced the concept of intrinsic spin because there is a fundamental relationship between the wavefunction of a system of identical particles and the spin of the component particles. Specifically, the wavefunction of a system of identical particles with integral spin $(0, 1, 2, \ldots)$ has even parity under exchange of two of the particles, and if the particles have non-integral spin $(1/2, 3/2, 5/2, \ldots)$ then the wavefunction has odd parity under exchange. That is,

$$P_{12}\Psi = \Psi \text{ for integer spins, and } P_{12}\Psi = -\Psi \text{ for non-integer spins}$$

where $P_{12}$ denotes the interchanging of identical particles 1 and 2. These conditions are referred to as symmetry conditions. Particles with integer spins are called bosons, particles with non-integer spins are called fermions.

Consider a scattering experiment with two identical particles. There is nothing to say that solving the scattering equations is guaranteed to give a wavefunction that satisfies the appropriate symmetry condition. However, we note that because of the identity of the particles, if $\Phi$ is a solution of the scattering equations, $P_{12}\Phi$ will be also. Therefore, we can symmetrise our solution by setting $\Psi = \Phi + P_{12}\Phi$ for bosons, and $\Psi = \Phi - P_{12}\Phi$ for fermions. It is easily checked then that $\Psi$ obeys the appropriate symmetry condition, so all we have really done is apply a particular boundary condition stipulating that the wavefunction must have the correct symmetry.

## 6.3 A Three-Body Scattering Problem

In this section we shall consider the scattering equations pertaining to a system of three particles, two of which are identical spin-$1/2$ fermions (labelled 1 and 2) which we shall assume

to have mass $1/2$, and particle 3 which is spinless and very heavy by comparison. The inital deployment of the particles is that of particle 1 incident on a bound state $(2,3)$. We might think of this system as an electron scattering off a hydrogen atom. However, for analytical convenience, we shall later make the approximation that all the potential interactions are separable, $V_1$ and $V_2$ being attractive and $V_3$ repulsive. Because particles 1 and 2 are identical, it is clear that the *functional forms* of $V_1$ and $V_2$ are identical. That is,

$$V_1(x_\alpha) = V_2(x_\alpha) \qquad (\alpha = 1,2,3). \tag{6.7}$$

We also expect for the same reason that the total coordinate wavefunctions should have the same functional forms in the Jacobi coordinates of particles 1 and 2. That is,

$$\phi^+_{\mathbf{q}}(\mathbf{X}_1) = \phi^+_{\mathbf{q}}(\mathbf{X}_2) \tag{6.8}$$

(we have dropped the subscript $n$ because separable potentials may only have one bound state). The Jacobi coordinates have the following simple forms for this system:

$$\begin{array}{cccc} \mathbf{x}_1 = \mathbf{r}_2, & \mathbf{y}_1 = -\mathbf{r}_1 & & \mathbf{p}_1 = \mathbf{k}_2 & \mathbf{q}_1 = -\mathbf{k}_1 \\ \mathbf{x}_2 = -\mathbf{r}_1 & \mathbf{y}_2 = -\mathbf{r}_2 & ; & \mathbf{p}_2 = -\mathbf{k}_1 & \mathbf{q}_2 = -\mathbf{k}_2 \\ \mathbf{x}_3 = \dfrac{\mathbf{r}_1 - \mathbf{r}_2}{\sqrt{2}} & \mathbf{y}_3 = \dfrac{\mathbf{r}_1 + \mathbf{r}_2}{\sqrt{2}} & & \mathbf{p}_3 = \dfrac{\mathbf{k}_1 - \mathbf{k}_2}{\sqrt{2}} & \mathbf{q}_3 = \dfrac{\mathbf{k}_1 + \mathbf{k}_2}{\sqrt{2}} \end{array}. \tag{6.9}$$

Let us now consider the spin wavefunction of the system. The spin Hilbert space is just $\ell^2(2) \otimes \ell^2(2)$ which is easily seen to be isomorphic to $\ell^2(4)$ (we have of course neglected the third particle as it is spinless). Now, it is well known that the total spin, $S$, of a two spin-$1/2$ particle system can be 1 or 0 depending upon whether the spins of the individual particles are aligned or not. It is also well known [22] that the spin wavefunction of the system will be symmetric when $S = 1$ and antisymmetric when $S = 0$. Therefore, since the system consists of identical fermions (so the total wavefunction must be antisymmetric), we conclude that the coordinate wavefunction will be antisymmetric when $S = 1$ and symmetric when $S = 0$. In terms of our interchanging notation ($P_{12}$), this becomes

$$P_{12}\phi^+_{\mathbf{q}}(\mathbf{X}_\alpha) = (-1)^S \phi^+_{\mathbf{q}}(\mathbf{X}_\alpha) \qquad (\alpha = 1,2,3). \tag{6.10}$$

Let us now apply this result to the differential Faddeev equations (5.23). These may be rearranged to give

$$\left[E + \nabla^2_{\mathbf{X}}\right] \phi^{(\alpha)}(\mathbf{X}_\alpha) = V_\alpha(x_\alpha) \sum_{\gamma=1}^{3} \phi^{(\gamma)}(\mathbf{X}_\gamma) = V_\alpha(x_\alpha)\, \phi^+_{\mathbf{q}}(\mathbf{X}_\alpha).$$

This is a differential equation for $\phi^{(\alpha)}$, the homogeneous solution of which is a free plane wave. However, it is clear (see [12] for a rigorous justification) that one boundary condition we should impose upon the $\phi^{(\alpha)}$ is that they asymptotically approach the *bound plane wave* $\phi_{\mathbf{q}_\alpha}$ (defined in section 5.3.4). The homogeneous solution does not satisfy this condition (we are considering a $1,(2,3)$ process) so we need only consider the particular solution of this equation. Therefore,

$$\phi^{(\alpha)}(\mathbf{X}_\alpha) = \lim_{\varepsilon \to 0^+} \int_{\mathbb{R}^6} G_0(\mathbf{X}_\alpha, \mathbf{X}'_\alpha; E + i\varepsilon) V_\alpha(x'_\alpha)\, \phi^+_{\mathbf{q}}(\mathbf{X}'_\alpha)\, d\mathbf{X}'_\alpha. \tag{6.11}$$

For the case $\alpha = 1$, we interchange particles 1 and 2 to get

$$\begin{aligned} P_{12}\phi^{(1)}(\mathbf{X}_1) &= P_{12}\left[\lim_{\varepsilon \to 0^+} \int_{\mathbb{R}^6} G_0(\mathbf{X}_1, \mathbf{X}'_1; E + i\varepsilon) V_1(x'_1)\, \phi^+_{\mathbf{q}}(\mathbf{X}'_1)\, d\mathbf{X}'_1\right] \\ &= \lim_{\varepsilon \to 0^+} \int_{\mathbb{R}^6} G_0(\mathbf{X}_2, \mathbf{X}'_2; E + i\varepsilon) V_1(x'_2)\, (-1)^S \phi^+_{\mathbf{q}}(\mathbf{X}'_2)\, d\mathbf{X}'_2 \\ &= \lim_{\varepsilon \to 0^+} (-1)^S \int_{\mathbb{R}^6} G_0(\mathbf{X}_2, \mathbf{X}'_2; E + i\varepsilon) V_2(x'_2)\, \phi^+_{\mathbf{q}}(\mathbf{X}'_2)\, d\mathbf{X}'_2 \end{aligned}$$

using equations 6.7 and 6.8 and the fact that the free Green's function has the same functional form in Jacobi coordinates 1 and 2. Comparing with equation 6.11, we see that this is just

$$P_{12}\phi^{(1)}(\mathbf{X}_1) = (-1)^S \phi^{(2)}(\mathbf{X}_2).$$

This result is extremely important because it allows us to rewrite our decomposition of the full wavefunction as

$$\phi^+_{\mathbf{q}}(\mathbf{X}) = \phi^{(1)}(\mathbf{X}_1) + \phi^{(2)}(\mathbf{X}_2) + \phi^{(3)}(\mathbf{X}_3) = \left[1 + (-1)^S P_{12}\right] \phi^{(1)}(\mathbf{X}_1) + \phi^{(3)}(\mathbf{X}_3) \quad (6.12)$$

and therefore reduce our differential Faddeev equations to a set of *two* coupled differential equations:

$$\begin{aligned} \left[E + \nabla^2_{\mathbf{X}} - V_1(x_1)\right] \phi^{(1)}(\mathbf{X}_1) &= V_1(x_1) \left[(-1)^S P_{12}\phi^{(1)}(\mathbf{X}_1) + \phi^{(3)}(\mathbf{X}_3)\right] \\ \left[E + \nabla^2_{\mathbf{X}} - V_3(x_3)\right] \phi^{(3)}(\mathbf{X}_3) &= V_3(x_3) \left[1 + (-1)^S P_{12}\right] \phi^{(1)}(\mathbf{X}_1). \end{aligned} \quad (6.13)$$

We have not made the separable approximation yet. However, we recall that the separable two-body problem was easily solved as an integral equation in momentum space. Let us therefore investigate what happens when we convert this set of differential equations into integral equations. We note that the first equation has a bound plane wave as the homogeneous solution:

$$\left[E + \nabla^2_{\mathbf{X}} - V_1(x_1)\right] \phi_{\mathbf{q}_1}(\mathbf{X}_1) = 0$$

whereas the second has no homogeneous solution since $V_3$ does not support a bound state. Therefore, we have the integral equations

$$\begin{aligned} \phi^{(1)}(\mathbf{X}_1) = \phi_{\mathbf{q}_1}(\mathbf{X}_1) + \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}^6} G_1\left(\mathbf{X}_1, \mathbf{X}_1'; E + i\varepsilon\right) V_1\left(x_1'\right) \times \\ \times \left[(-1)^S P_{12}\phi^{(1)}\left(\mathbf{X}_1'\right) + \phi^{(3)}\left(\mathbf{X}_3'\right)\right] d\mathbf{X}_1' \end{aligned} \quad (6.14)$$

$$\phi^{(3)}(\mathbf{X}_3) = \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}^6} G_3\left(\mathbf{X}_3, \mathbf{X}_3'; E + i\varepsilon\right) V_3\left(x_3'\right) \left[1 + (-1)^S P_{12}\right] \phi^{(1)}\left(\mathbf{X}_1'\right) d\mathbf{X}_3'.$$

where $G_\alpha(\mathbf{X}_\alpha, \mathbf{X}_\alpha'; E)$ is the kernel of the operator $G_\alpha(E) = (E - H_0 - V_\alpha)^{-1}$.

Let us now Fourier transform these equations so that we can work in momentum space. Since

$$\widehat{\phi_{\mathbf{q}_1}}\left(\mathbf{P}_1'\right) = \frac{\widehat{\chi_1}(\mathbf{p}_1')}{(2\pi)^{3/2}} \delta\left(\mathbf{q}_1 - \mathbf{q}_1'\right),$$

we will now be working in a distributional setting, though this is not particularly troublesome. The operators $G_\alpha$ and $V_\alpha$ have complicated forms in momentum space, so we use the identity $G_\alpha V_\alpha = G_0 \tau_\alpha$ (equation 5.17) where $\tau_\alpha$ is the two-body $\tau$-operator defined in section 5.3.2. Our equations transform to

$$\begin{aligned} \widehat{\phi^{(1)}}\left(\mathbf{p}_1', \mathbf{q}_1'\right) = \widehat{\phi_{\mathbf{q}_1}}\left(\mathbf{p}_1', \mathbf{q}_1'\right) + \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}^3} \frac{\tau_1\left(\mathbf{p}_1', \mathbf{p}_1''; E_\varepsilon^{(1)}\right)}{E + i\varepsilon - q_1'^2 - p_1'^2} \times \\ \times \left[(-1)^S P_{12}\widehat{\phi^{(1)}}\left(\mathbf{p}_1'', \mathbf{q}_1'\right) + \widehat{\phi^{(3)}}\left(\frac{\mathbf{p}_1'' + \mathbf{q}_1'}{-\sqrt{2}}, \frac{\mathbf{q}_1' - \mathbf{p}_1''}{\sqrt{2}}\right)\right] d\mathbf{p}_1'' \end{aligned} \quad (6.15)$$

$$\widehat{\phi^{(3)}}\left(\mathbf{p}_3', \mathbf{q}_3'\right) = \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}^3} \frac{\tau_3\left(\mathbf{p}_3', \mathbf{p}_3''; E_\varepsilon^{(3)}\right)}{E + i\varepsilon - q_3'^2 - p_3'^2} \left[1 + (-1)^S P_{12}\right] \widehat{\phi^{(1)}}\left(\frac{\mathbf{q}_3' - \mathbf{p}_3''}{\sqrt{2}}, \frac{\mathbf{q}_3' + \mathbf{p}_3''}{-\sqrt{2}}\right) d\mathbf{p}_3''$$

where we have used the explicit forms (6.9) of the Jacobi coordinates for this system. Notice that the integration is only over three dimensions - in the coordinate representation, we were facing six-dimensional integrals. The price we pay for this simplification is of course having such complicated arguments in the component wavefunctions.

We now make our separable approximation. Recall that for separable potentials, the two-body $\tau$-operators have kernels given by equation 6.5:

$$\tau_\alpha\left(\mathbf{k},\mathbf{k}';E\right)=\frac{\lambda_\alpha\widehat{a_\alpha}\left(\mathbf{k}\right)\overline{\widehat{a_\alpha}\left(\mathbf{k}'\right)}}{\Delta_\alpha\left(E\right)}\quad;\quad\Delta_\alpha\left(E\right)=1-\lambda_\alpha\int_{\mathbb{R}^3}\frac{\left|\widehat{a_\alpha}\left(\mathbf{k}''\right)\right|^2}{E-k''^2}d\mathbf{k}''$$

where $a_\alpha\left(\mathbf{r}\right)$ is the form factor for $V_\alpha$ and $\lambda_\alpha$ represents the strength of that interaction. Substituting this into our momentum space equations (changing to the appropriate Jacobi coordinates) gives

$$\widehat{\phi^{(1)}}\left(\mathbf{p}_1',\mathbf{q}_1'\right)=\widehat{\phi_{\mathbf{q}_1}}\left(\mathbf{p}_1',\mathbf{q}_1'\right)+\lim_{\varepsilon\to0^+}\frac{\lambda_1\widehat{a_1}\left(\mathbf{p}_1'\right)}{\left(E+i\varepsilon-q_1'^2-p_1'^2\right)\Delta_1\left(E+i\varepsilon-q_1'^2\right)}\times$$
$$\times\int_{\mathbb{R}^3}\overline{\widehat{a_1}\left(\mathbf{p}_1''\right)}\left[\left(-1\right)^SP_{12}\widehat{\phi^{(1)}}\left(\mathbf{p}_1'',\mathbf{q}_1'\right)+\widehat{\phi^{(3)}}\left(\frac{\mathbf{p}_1''+\mathbf{q}_1'}{-\sqrt{2}},\frac{\mathbf{q}_1'-\mathbf{p}_1''}{\sqrt{2}}\right)\right]d\mathbf{p}_1''$$

$$\widehat{\phi^{(3)}}\left(\mathbf{p}_3',\mathbf{q}_3'\right)=\lim_{\varepsilon\to0^+}\frac{\lambda_3\widehat{a_3}\left(\mathbf{p}_3'\right)}{\left(E+i\varepsilon-q_3'^2-p_3'^2\right)\Delta_3\left(E+i\varepsilon-q_3'^2\right)}\times$$
$$\times\int_{\mathbb{R}^3}\overline{\widehat{a_3}\left(\mathbf{p}_3''\right)}\left[1+\left(-1\right)^SP_{12}\right]\widehat{\phi^{(1)}}\left(\frac{\mathbf{q}_3'-\mathbf{p}_3''}{\sqrt{2}},\frac{\mathbf{q}_3'+\mathbf{p}_3''}{-\sqrt{2}}\right)d\mathbf{p}_3''.$$

Let us now substitute into these equations form factors analogous to those we derived in section 6.1.2. That is, we follow equation 6.6 and let

$$\begin{aligned}a_1\left(\mathbf{x}_1\right)&=\frac{e^{-\Lambda x_1}}{x_1}\quad\Rightarrow\quad\widehat{a}_1\left(\mathbf{p}_1\right)=\sqrt{\frac{2}{\pi}}\frac{1}{\Lambda^2+p_1^2}\\\text{and }a_3\left(\mathbf{x}_3\right)&=\frac{e^{-\Lambda x_3}}{x_3}\quad\Rightarrow\quad\widehat{a}_3\left(\mathbf{p}_3\right)=\sqrt{\frac{2}{\pi}}\frac{1}{\Lambda^2+p_3^2}\end{aligned}$$

where $\Lambda>0$, and let $\lambda=\lambda_3=-\lambda_1>0$ (corresponding to the identical particles repelling one another and unlike particles attracting one another). We therefore have that

$$\lim_{\varepsilon\to0^+}\Delta_\alpha\left(E+i\varepsilon-q_\alpha^2\right)=1+\frac{2\pi\lambda_\alpha}{\Lambda\left(\Lambda-i\sqrt{E-q_\alpha^2}\right)^2}$$

where $\sqrt{E-q_\alpha^2}=i\sqrt{q_\alpha^2-E}$ if $E-q_\alpha^2<0$.

Substitution then gives the final form for our coupled equations:

$$\widehat{\phi^{(1)}}\left(\mathbf{p}_1',\mathbf{q}_1'\right)=\widehat{\phi_{\mathbf{q}_1}}\left(\mathbf{p}_1',\mathbf{q}_1'\right)-\Xi_1\left(\mathbf{p}_1',\mathbf{q}_1'\right)\times$$
$$\times\int_{\mathbb{R}^3}\frac{\left(-1\right)^SP_{12}\widehat{\phi^{(1)}}\left(\mathbf{p}_1'',\mathbf{q}_1'\right)+\widehat{\phi^{(3)}}\left(\frac{\mathbf{p}_1''+\mathbf{q}_1'}{-\sqrt{2}},\frac{\mathbf{q}_1'-\mathbf{p}_1''}{\sqrt{2}}\right)}{\Lambda^2+p_1''^2}d\mathbf{p}_1''$$

$$\widehat{\phi^{(3)}}\left(\mathbf{p}_3',\mathbf{q}_3'\right)=\Xi_3\left(\mathbf{p}_3',\mathbf{q}_3'\right)\int_{\mathbb{R}^3}\frac{\left[1+\left(-1\right)^SP_{12}\right]\widehat{\phi^{(1)}}\left(\frac{\mathbf{q}_3'-\mathbf{p}_3''}{\sqrt{2}},\frac{\mathbf{q}_3'+\mathbf{p}_3''}{-\sqrt{2}}\right)}{\Lambda^2+p_3''^2}d\mathbf{p}_3''$$

where

$$\Xi_\alpha\left(\mathbf{p}_\alpha',\mathbf{q}_\alpha'\right)=\frac{2\lambda}{\pi\left(\Lambda^2+p_\alpha'^2\right)\left(E-p_\alpha'^2-q_\alpha'^2\right)\left[1+\frac{2\pi\lambda}{\Lambda\left(\Lambda-i\sqrt{E-q_\alpha'^2}\right)^2}\right]}.$$

This is about as far as our analysis can take us. We now have a set of two coupled, three-dimensional integral equations for the component wavefunctions, which do not have singular kernels (although the $\Xi_\alpha$ do have a singularity). In fact, because $\widehat{\phi^{(3)}}$ is only dependent upon $\widehat{\phi^{(1)}}$, the second equation can in principle be substituted into the first, leading to one very complicated six-dimensional equation in $\widehat{\phi^{(1)}}$. However we proceed, the equations can now be subjected to angular analysis and then solved numerically on a computer. The compactness of the original Faddeev equations guarantees that a unique solution will exist.

Once we have ascertained the wavefunction $\phi^+_{\mathbf{q}_\beta}(\mathbf{X})$, we can calculate the T-matrix appropriate to a scattering event initally in channel $\beta$ and finally in channel $\alpha$ using a generalisation of equation 4.22 [45]:

$$t_{\beta\to\alpha}\left(\mathbf{P},\mathbf{P}'\right) = \int_{\mathbb{R}^6} \overline{\phi_f\left(\mathbf{x}_\alpha,\mathbf{y}_\alpha\right)} V^{(\alpha)}(\mathbf{X})\,\phi^+_{\mathbf{q}_\beta}(\mathbf{X})\,d\mathbf{X}$$

where $\phi_f$ is the asymptotic eigenfunction appropriate for channel-$\alpha$, and $V^{(\alpha)}(\mathbf{X})$ are all the potentials which become negligible in the final channel ($V^{(\alpha)} = H - H^\alpha$). For our calculation, $\beta = 1$ as the initial deployment was a $1,(2,3)$ system. The label $\alpha$ may take the values 0, 1 or 2, corresponding to break-up, elastic scattering and rearrangement processes respectively. Channel-3 is not possible ('open') because a $(1,2)$ bound state is not possible. Note that because separable potentials can only support one bound state, inelastic scattering is not possible. It is also apparent that because particles 1 and 2 are identical, we cannot distinguish between elastic scattering and rearrangement (channels 1 and 2).

Explicitly then, we would calculate

$$\begin{aligned}
t_{1\to1}\left(\mathbf{P},\mathbf{P}'\right) &= \int_{\mathbb{R}^6} \overline{\phi_{\mathbf{q}_1}(\mathbf{X}_1)}\left[V_2(x_2)+V_3(x_3)\right]\phi^+_{\mathbf{q}_1}(\mathbf{X})\,d\mathbf{X},\\
t_{1\to2}\left(\mathbf{P},\mathbf{P}'\right) &= \int_{\mathbb{R}^6} \overline{\phi_{\mathbf{q}_2}(\mathbf{X}_2)}\left[V_1(x_1)+V_3(x_3)\right]\phi^+_{\mathbf{q}_1}(\mathbf{X})\,d\mathbf{X}\\
\text{and}\quad t_{1\to0}\left(\mathbf{P},\mathbf{P}'\right) &= \int_{\mathbb{R}^6} \overline{\phi_{\mathbf{P}}(\mathbf{X})}\left[V_1(x_2)+V_2(x_2)+V_3(x_3)\right]\phi^+_{\mathbf{q}_1}(\mathbf{X})\,d\mathbf{X}
\end{aligned}$$

in whatever Jacobi coordinates are appropriate. The $\phi_{\mathbf{q}_\alpha}$ are of course bound plane waves, and the $\phi_{\mathbf{P}}$ is the free plane wave appropriate for the break-up channel.

The relationship to the experimental cross-section is a little more complicated than that of two-body scattering. Each final channel $\alpha$ gives rise to a differential cross-section that is proportional to $\left|t_{1\to\alpha}(\mathbf{P},\mathbf{P}')\right|^2$. However, because the momenta and the reduced masses of any two-body pairs present can all vary, the proportionality constants are different for each channel. Also, in the break-up channel we can detect more than one particle so there are several differential cross-sections corresponding to each type of measurement we choose to make. Explicit forms for all these quantities may be found in [45] or [35]. We note finally that once these are calculated, they may be integrated to get a total channel cross-section, $\sigma_{1\to\alpha}$. Because we cannot distinguish between elastic scattering and rearrangement in this process, the elastic cross-section is the sum of $\sigma_{1\to1}$ and $\sigma_{1\to2}$. The total cross-section for the scattering process is then the sum of the elastic cross-section and the break-up cross-section $\sigma_{1\to0}$.

# Chapter 7

# Conclusion

> "*Quantum theory - the dreams stuff is made of...*"
> Unknown

We have discussed at some length a rigorous treatment of the fundamental mathematical aspects of quantum scattering theory. Our treatment was based on the *spectral theorem for unbounded self-adjoint operators* which was proven here following the original work of *Von Neumann*. To discuss scattering theory appropriately, the position, momentum and energy operators were introduced. Particular attention was paid to the results of *Kato* concerning the self-adjointness of the Hamiltonian operator, using the concept of relative bounds.

Using these results, it was then possible to rigorously formulate the equations of scattering theory. The Green's operators, wave operators and the scattering operator were introduced in the context of two-body time dependent scattering theory and their properties and importance were briefly surveyed. The time independent definitions of the wave operators were established following *Amrein et al.* This led to the standard equations of two-body time independent scattering theory via the *eigenfunction expansion* technique. However, in order to make the derivations rigorous but reasonably straight-forward, the operator equations were only considered to act upon a "part" of the Hilbert space for which the operators had "nice" representations. We did not need to presume (as for instance, [38] does) that these representations hold over the whole Hilbert space.

We then considered generalising these results to a three-body scattering problem. We briefly indicated how the theory can be easily extended to this case, although the corresponding broadening of the three-body theory was found to be not strictly rigorous. Nevertheless, examination showed that these three-body equations were found to be unsatisfactory for (numerical) computation, unlike the two-body equations. To cover this deficiency, we followed the original work of *Faddeev*, detailing his decomposition method and discussing why this technique might be expected to produce more satisfactory equations. We then used his decomposition to present our own derivation of the *differential Faddeev equations* which are stated in [15].

As an application of this formulation of three-body scattering theory, we then derived a set of equations for a particular three-body problem incorporating the effects of intrinsic particle spin and identical particles. However, for convenience we assumed that the potential interactions between the particles were *separable*, a form which is known to be more amenable to analytic results. This assumption allowed us to explicitly evaluate some of the terms and therefore to better understand the equation structure.

Future work would of course concentrate on solving these equations. This would involve first subjecting our coupled set of equations to an angular analysis. This standard procedure is based on the role of the *angular momentum operators* in scattering theory which was not discussed in this thesis (see [35] for instance). After this is achieved, the result would then be solved numerically on a computer. The solution obtained would then be of value as a comparison for evaluating the performance (and practicality) of other three-body scattering

formulations, as well as being of interest as a three-body scattering wavefunction in its own right.

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