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Asymptotic observables for quantum Hamiltonians with external fields

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Declaration

I hereby declare that this thesis has not been and will not be submitted in whole or in part to another University for the award of any other degree.

Most of the work presented in this thesis was done in collaboration with my supervisor Professor Michael Melgaard. The material contained in this thesis is original and my own work except where otherwise stated.

Signature, May 7, 2021

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Waleed Hamali, Doctor of Philosophy

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Summary

The description of the large-time asymptotic behaviour of scattering states via selected time-dependent observables has proven tremendously important in quantum mechanical scattering, in particular for establishing asymptotic completeness. The thesis presents new results for such asymptotic observables for a class of quantum Hamiltonians with external fields. The first part of the thesis presents the necessary mathematical theory and methods used to establish the results including an introduction to scattering theory (physics level), elements of linear operator theory, elements of mathematical scattering theory (decomposition of the spectrum and characterisation of scattering states, the Møller wave operators etc), and a classic result on asymptotic completeness. The second part presents the new results with detailed proofs.

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Chapter 1

Introduction

In Quantum Mechanics a particle, whose position in classical mechanics is described by a point in the Euclidean space $\mathbb{R}^d$, is described by a complex-valued function $\Psi \in L^2(\mathbb{R}^d;\mathbb{C})$, which is called the wave function of the particle. The modulus-square of the wave function, i.e. $|\Psi(\boldsymbol{x})|^2$, is interpreted as a density function, which equals the probability for finding the particle in a neighborhood of a point $\boldsymbol{x} \in \mathbb{R}^d$. As a consequence, $\|\Psi\|_{L^2(\mathbb{R}^d;\mathbb{C})} = 1$. If the state of the particle at time $t = 0$ is given by $\Psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$, then the state of the particle at time t equals

$$\Psi(t) = U(t)\Psi_0,$$

where $U(t)$ is a strongly continuous one-parameter group of unitary operators on $L^2(\mathbb{R}^d)$. According to Stone's theorem one has that

$$U(t) = e^{-itH},$$

where H is a self-adjoint operator on $L^2(\mathbb{R}^d)$, which is referred to as the Hamilton operator of the system. In the case where $\Psi_0 \in \mathrm{Dom}\,(H)$, $\Psi(t) = \exp(-itH)\Psi_0$ is strongly differentiable and obeys the differential equation

$$\partial_t \Psi(t) = -iH\Psi(t), \quad \Psi(0) = \Psi_0,$$

which is called the time-dependent Schrödinger equation. In non-relativistic Quantum Mechanics the Hamilton operator is typically the closure of an essentially self-adjoint differential operator of the type

$$-\frac{1}{2m}\Delta + V(\boldsymbol{x}), \tag{1.1}$$

where m is the mass of the particle, Δ is the Laplace operator and $V(\boldsymbol{x})$ is a real-valued function which acts as a multiplication operator on $L^2(\mathbb{R}^d)$. When H takes this expression, it is known as a Schrödinger operator; an exception is the special case $V = 0$, where H describes a free particle. In that case H is called the free Hamiltonian or free Hamilton operator, and it is denoted by H_0.

The Schrödinger operator H describes the energy of the system and if the particle is in a state Ψ, then the expectation of the energy equals

$$E = \int_{\mathbb{R}^d} \overline{\Psi(\boldsymbol{x})}(H\Psi)(\boldsymbol{x})\, d\boldsymbol{x} = \langle \Psi, H\Psi \rangle_{L^2}.$$

Here $\langle \cdot, \cdot \rangle$ denotes the inner product on $L^2(\mathbb{R}^d; \mathbb{C})$. In a similar way, the multiplication operator induced by $\boldsymbol{x}$ and the differential operator $\boldsymbol{p} = -i\nabla$ describe the position and the momentum of the particle, respectively. Notice that the expectation of the kinetic energy is

$$T = \langle \Psi, H_0\Psi \rangle = -\frac{1}{2m} \int \overline{\Psi(\boldsymbol{x})}(\Delta\Psi)(\boldsymbol{x})\, d\boldsymbol{x} = \frac{1}{2m} \int |(\boldsymbol{p}\Psi)(\boldsymbol{x})|^2\, d\boldsymbol{x}.$$

Hence, in (1.1) the kinetic energy is represented by $-\Delta/2m$, while $V(\boldsymbol{x})$ represents the potential energy. We shall restrict ourselves to two-body systems and therefore the potential $V(\boldsymbol{x})$ is a function of the relative position $\boldsymbol{x}$ of the two particles, $-\Delta/2m$ is the kinetic energy given by the relative velocity of the particles, and m is the reduced mass of the system.

Let $\mathcal{H}_{\mathrm{p}}(H)$ be the smallest closed subspace of $\mathcal{H} = L^2(\mathbb{R}^d)$ which contains all the eigenvectors of H. If $\Psi \in \mathcal{H}_{\mathrm{p}}(H)$ then, at any time, $\exp(-itH)\Psi$ will be "localized" to a certain part of the space, or "bounded within" a certain part of the space. More precisely: for any $\epsilon > 0$ there exists a $r > 0$ such that for all times (see also Chapter 4)

$$\int_{|\boldsymbol{x}| \geq r} |e^{-itH}\Psi(\boldsymbol{x})|^2\, d\boldsymbol{x} \leq \epsilon.$$

This agrees with the physical intuition one has about an eigenvector; for this reason $\Psi \in \mathcal{H}_{\mathrm{p}}(H)$ is also called a bound state. If, on the other hand, $\Psi \in \mathcal{H}_{\mathrm{p}}(H)^{\perp} := \mathcal{H}_{\mathrm{c}}(H)$, where the latter is called the continuous subspace, then $\exp(-itH)\Psi$ leaves every ball around the origin as times goes by (for the precise statement, see Chapter 4). Therefore such a vector Ψ is called a scattering state.

In the case where $V(\boldsymbol{x}) \longrightarrow 0$ as $|\boldsymbol{x}| \to \infty$, one intuitively expects that a particle which is not bounded, will eventually move as a free particle: along a straight line and with constant speed. In other words, if $\Psi \in \mathcal{H}_{\rm c}(H)$ is a scattering state, then one intuitively expects that there exists a state $\Psi_+ \in \mathcal{H}$ such that

$$\lim_{t\to\infty} \|e^{-itH}\Psi - e^{-itH_0}\Psi_+\| = 0 \tag{1.2}$$

and, similarly, a state $\Psi_- \in \mathcal{H}$ corresponding to the case where $t \to -\infty$. In fact, one expects that for any vector $\Psi_+ \in \mathcal{H}$ there exists a scattering state $\Psi \in \mathcal{H}_{\rm c}(H)$ such that (1.2) holds. Thus it is natural to consider the family of operators

$$W(t) = e^{itH}e^{-itH_0} \tag{1.3}$$

and investigate whether the strong limits

$$W_\pm = \operatorname*{s-lim}_{t\to\pm\infty} W(t) \tag{1.4}$$

exist. The operators $W_\pm$ are called the Møller wave operators.

One of the main goals of scattering theory is to prove that the wave operators exist. Another goal has already been indicated by the afore-mentioned intuitive argument. If Ψ is not a bound state ($\Psi \perp \mathcal{H}_{\rm p}(H)$), then one expects that $\exp(-itH)\Psi$ will look like a free state asymptotically, i.e., there exists $\Psi_+ \in \mathcal{H}$ such that (1.2) holds. A bound state, on the other hand, will never look like a free state, i.e., (1.2) will not be valid for any $\Psi_+ \in \mathcal{H}$, if $\Psi \in \mathcal{H}_{\rm p}(H)$. This property is called asymptotic completeness.

Definition 1.0.1 *The system described by the Schrödinger operator H is said to be asymptotically complete if the Møller wave operators $W_\pm$ exist and* $\operatorname{Ran}(W_\pm) = \mathcal{H}_{\rm c}(H)$*. It is also said that $W_\pm$ are complete.*

When one shows completeness of $W_\pm$, it is sufficient to show existence of the limit

$$\lim_{t\to\infty} e^{itH_0}e^{-itH}\Psi$$

for all Ψ belonging to a dense subset of $\mathcal{H}_{\rm c}(H)$ because the operators $\exp(-itH)$ and $\exp(itH_0)$ are unitary.

As already indicated one can expect that the wave operators exist when H only differs a little bit, in some sense, from the free Hamiltonian H_0. For this reason one can say that the study of the wave operators is a branch of perturbation theory for linear operators. This is emphasized by the properties they have:

Theorem 1.0.2 *If the wave operators $W_\pm$ exist, then they are partial isometries with initial subspace $\mathcal{H}$ and final subspace* $\mathrm{Ran}\,(W_\pm)$*. One has* $\mathrm{Ran}\,(W_\pm) \subseteq \mathcal{H}_\mathrm{c}(H)$ *and* $\mathrm{Ran}\,(W_\pm)$ *reduces $\mathcal{H}$ (This notion and other relevant notions are explained in Chapter 3). In addition, the so-called intertwining relation holds; for a proof we refer to [18], p 530:*

$$HW_\pm \supseteq W_\pm H_0. \tag{1.5}$$

That $\mathrm{Ran}\,(W_\pm) \subseteq \mathcal{H}_\mathrm{c}(H)$ is a confirmation of the intuitive expectation that bound states will never look like free states. Since $\mathrm{Ran}\,(W_\pm)$ reduces H, one can define the restrictions, $H_\pm$, of H to $\mathrm{Ran}\,(W_\pm)$:

$$\mathrm{Dom}\,(H_\pm) = \mathrm{Dom}\,(H) \cap \mathrm{Ran}\,(W_\pm)\,;$$
$$H_\pm \Psi = H\Psi\,; \quad \Psi \in \mathrm{Dom}\,(H_\pm).$$

Since the wave operators are partial isometries, they can be considered as unitary mappings of $\mathcal{H}$ onto $\mathrm{Ran}\,(W_\pm)$ with $W_\pm^{-1} = W_\pm^*$. The intertwining relation (1.5) shows that $H_\pm$ is unitarily equivalent with H_0:

$$H_0 = W_\pm^* H_\pm W_\pm.$$

This is an important property of the wave operators and, for instance, it tells us that $\mathrm{spec}\,(H_\pm) = \mathrm{spec}\,(H_0)$ is absolutely continuous. If $W_\pm$ are complete, i.e., $\mathrm{Ran}\,(W_\pm) = \mathcal{H}_\mathrm{c}(H)$, then the conclusion is even stronger. In that case $H_\pm = H_\mathrm{c}$ with H_c being the restriction of H to $\mathcal{H}_\mathrm{c}(H)$, and one infers that H has no singular continuous spectrum; indeed, $\mathrm{spec}\,(H_\pm) = \mathrm{spec}\,(H_\mathrm{c}) = \mathrm{spec}_\mathrm{c}\,(H)$ which equals $\mathrm{spec}\,(H_0) = [0, \infty)$ which, as already noted, is absolutely continuous.

In this dissertation we derive results on propagation properties for Hamiltonians with external magnetic fields.

The description of the large-time asymptotic behaviour of scattering states via selected time-dependent observables has proven tremendously important in quantum mechanical scattering. For instance, for a Schrödinger operator H in $L^2(\mathbb{R}^d)$ and position operator $\boldsymbol{x}$, resp., momentum operator $\boldsymbol{p}$, one can show that

$$\left(\frac{\boldsymbol{x}}{t} - \boldsymbol{p}\right) e^{-itH}\Psi \longrightarrow 0, \tag{1.6}$$

as $|t| \to \infty$, provided $\Psi \in \mathcal{H}_{\mathrm{c}}(H)$; the continuous spectral subspace of the Hamiltonian H. This result, due to Enss [9] (see also [2, 8]), can be interpreted as follows: when the scattering or interaction between the particle and the scattering has taken place (i.e. $|t|$ is large), then the average velocity $\boldsymbol{x}/t$ of the particle and its momentum $\boldsymbol{p}$ will almost coincide. This agrees with the physical intuition.

A consequence of (1.6), which has proven important for long-range interactions and many-particle systems (see, e.g., [10]), says that if $j \in C_0^\infty(\mathbb{R}^d)$ then, for any scattering state $\Psi \in \mathcal{H}_{\mathrm{c}}(H)$,

$$\left\{ j\left(\frac{\boldsymbol{x}}{t}\right) - j(\boldsymbol{p}) \right\} e^{-itH}\Psi \longrightarrow 0, \tag{1.7}$$

as $|t| \to \infty$. Physically, this fact can be interpreted as follows: after the interaction with the scattering centre that part of the state which has momenta localized in the support of $j(\cdot)$ will be spatial localized in the support of $j(\cdot/t)$.

The main theorem, established for quantum Hamiltonians $H(\mathcal{A})$ for a class of vector potentials $\mathcal{A}$ (see Chapter 7 for details) asserts:

Theorem 1.0.3 *For $\Psi \in \mathcal{H}_c(H(\mathcal{A}))$ and for any $f \in C_0^\infty(\mathbb{R}^d)$*

$$\|\{f(\frac{\boldsymbol{x}}{t}) - f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi\|_{\mathcal{H}} \longrightarrow 0 \tag{1.8}$$

We also give some generalizations of this result.

Part I

Scattering theory

Chapter 2

Introduction to scattering theory

2.1 Scattering phenomena

Scattering theory is important as it underpins one of the most ubiquitous tools in physics. Almost everything we know about nuclear and atomic physics has been discovered by scattering experiments, e.g. Rutherford's discovery of the nucleus, the discovery of sub-atomic particles (such as quarks), etc. In low energy physics, scattering phenomena provide the standard tool to explore solid state systems, e.g. neutron, electron, x-ray scattering, etc. As a general topic, it therefore remains central to any advanced course on quantum mechanics.

In this introductory chapter, we briefly recall the general methodology (on the level of undergraduate physics) before we proceed to a more in-depth mathematically rigorous theory of scattering theory beginning in Chapter 3.

2.1.1 Background

In an idealized scattering experiment, a sharp beam of particles (A) of definite momentum $\boldsymbol{k}$ are scattered from a localized target (B). As a result of collision, several outcomes are possible:

$$A + B \longrightarrow \begin{cases} A + B \\ A + B^{*} \\ A + B + C \\ C \end{cases}$$

where $A + B \to A + B^{*}$ means inelastic scattering, i.e., the total kinetic energy is not conserved, in other words, the initial energy is not equal to final energy (state change), and $A + B \to C$ means inelastic or absorption, i.e., the final collision may not be same as initial particles, some particles may be created or disappears.

In high energy and nuclear physics, we are usually interested in deep inelastic processes. To keep our discussion simple, we will focus on elastic processes in which both the energy and particle number are conserved – although many of the concepts that we will develop are general.

2.1.2 Differential cross section

Both classical and quantum mechanical scattering phenomena are characterized by the scattering cross section, σ.

Consider a collision experiment in which a detector measures the number of particles per unit time, $N\, d\Omega$, scattered into an element of solid angle $d\Omega$ in direction (θ, ϕ). This number is proportional to the incident flux of particles, j_I defined as the number of particles per unit time crossing a unit area normal to direction of incidence. Collisions are characterised by the differential cross section defined as the ratio of the number of particles scattered into direction (θ, ϕ) per unit time per unit solid angle, divided by incident flux,

$$\frac{d\sigma}{d\Omega} = \frac{N}{j_I}$$

From the differential, we can obtain the total cross section by integrating over all solid angles

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \frac{d\sigma}{d\Omega}$$

The cross section, which typically depends sensitively on energy of incoming particles, has dimensions of area and can be separated into $\sigma_{elastic}, \sigma_{inelastic}, \sigma_{\text{abs}}$ and σ_{total}.

In the following, we will focus on elastic scattering where internal energies remain constant and no further particles are created or annihilated, e.g. low energy scattering of neutrons from protons. However, before turning to quantum scattering, let us consider classical scattering theory.

2.1.3 Classical theory

In classical mechanics, for a central potential, $V(r)$, the angle of scattering is determined by an impact parameter $b(\theta)$.

The number of particles scattered per unit time between θ and $\theta + d\theta$ is equal to the number of incident particles per unit time between b and $b + db$; see Figure 2.1. Therefore, for incident flux j_I, the number of particles scattered into the solid angle $d\Omega = 2\pi \sin\theta d\theta$ per unit time is given by

$$N d\Omega = 2\pi \sin\theta \, d\theta N = 2\pi b \, db j_I$$

i.e.

$$\frac{d\sigma(\theta)}{d\Omega} \equiv \frac{N}{j_I} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|$$

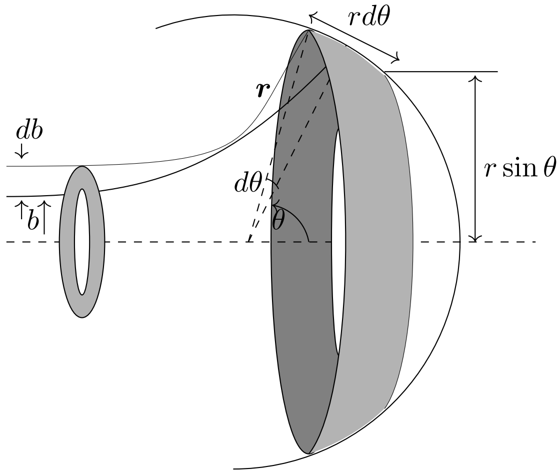

Figure 2.1: Number of particles scattered into solid angle per unit time.

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right| .$$

For elastic scattering from a hard (impenetrable) sphere (see Figure 2.2), we have that

$$b(\theta) = R \sin\alpha = R \sin\left(\frac{\pi - \theta}{2}\right) = -R\cos(\theta/2).$$

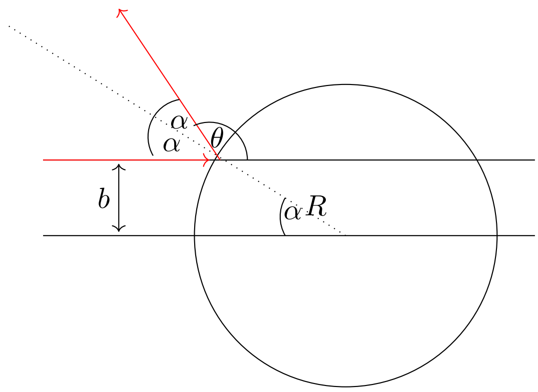

Figure 2.2: Illustration of elastic scattering from a hard (impenetrable) sphere.

As a result, we find that $\left|\frac{b}{\theta}\right| = \frac{R}{2}\sin(\theta/2)$ and

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{R^2}{4}$$

As expected, total scattering cross section is just $\int d\Omega \frac{d\sigma}{d\Omega} = \pi R^2$, the projected area of the sphere.

For classical Coulomb scattering,

$$V(r) = \frac{k}{r}$$

the particle follows a hyperbolic trajectory.

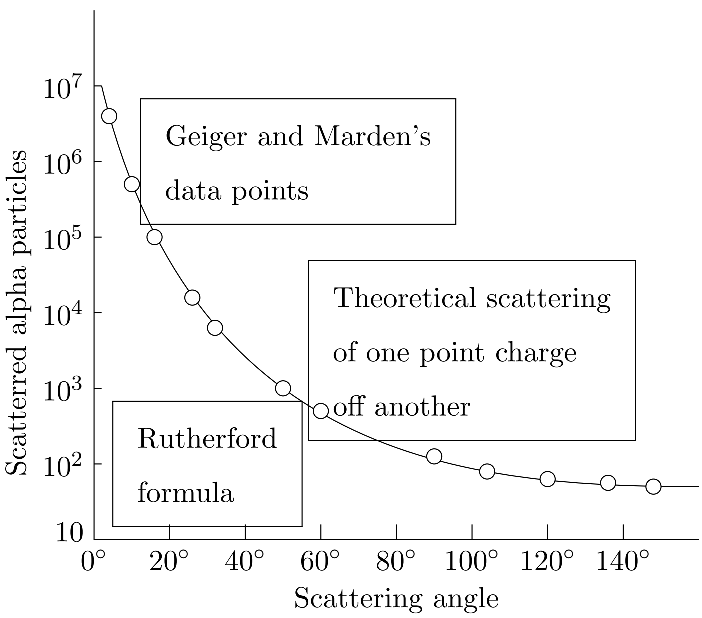

Figure 2.3: Classical Coulomb scattering.

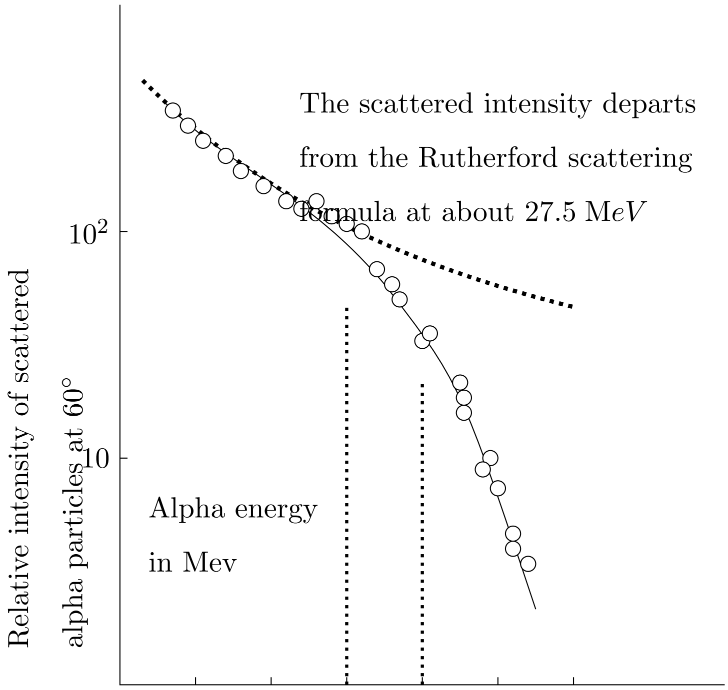

Figure 2.4: Classical Coulomb scattering.

In this case, a straightforward calculation yields the Rutherford formula:

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \frac{k^2}{16E^2}\frac{1}{\sin^4\theta/2}.$$

2.2 Scattering in Quantum Physics

Firstly, we consider the simplest scattering experiment: plane wave impinging on localized potential, $V(\boldsymbol{r})$, e.g. electron striking atom, or α particle a nucleus; see Figure 2.5. We have a flux of particles, all at the same energy, scattered from target and collected by detectors which measure angles of deflection.

In principle, if all incoming particles represented by wavepackets, the task is to solve time-dependent Schrödinger equation,

$$i\hbar\partial_t\Psi(\boldsymbol{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\Psi(\boldsymbol{r},t)$$

and find probability amplitudes for outgoing waves. However, if beam is "switched on" for times long as compared with "encounter-time", steady-state conditions apply. If wave-packet has well-defined energy (and hence momentum), may consider it a plane wave: $\Psi(\boldsymbol{r},t) = \psi(\boldsymbol{r})e^{-iEt/\hbar}$. Therefore, we seek solutions of time-independent Schrödinger

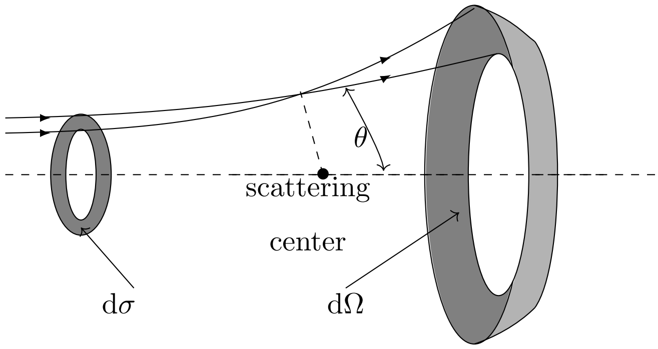

Figure 2.5: Scattering experiment, e.g., electron striking an atom.

equation,

$$E\psi(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r})$$

subject to boundary conditions that incoming component of wavefunction is a plane wave, $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ (cf. Section 2.2.1 below).

The energy of incoming particles equals $E = (\hbar\boldsymbol{k})^2/2m$ while the flux is given by

$$\boldsymbol{j} = -i\frac{\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*) = \frac{\hbar\boldsymbol{k}}{m}.$$

2.2.1 Examples of scattering in one spatial dimension

In one-dimension, interaction of plane wave, e^{ikx} , with localized target (see Figure 2.6) results in degree of reflection and transmission.

Both components of outgoing scattered wave are plane waves with wavevector $\pm k$ (energy conservation). Influence of potential encoded in complex amplitude of reflected and transmitted wave – fixed by time-independent Schrödinger equation subject to boundary conditions (flux conservation).

Consider the solutions of time-independent Schrödinger equation,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E\psi(r)$$

For any potential, there are essentially two different kinds of states we are interested in.

Bound states are states that are localized in some region of space. The wave funtions are

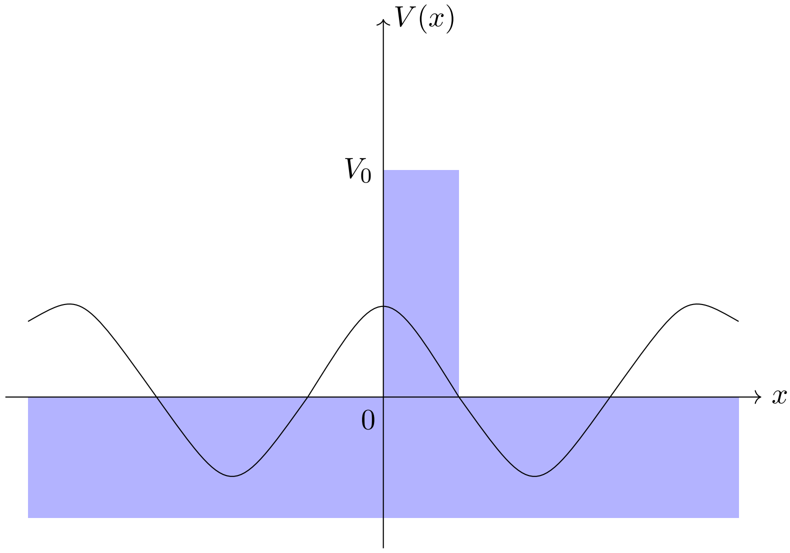

Figure 2.6: Plane wave interacting with localized target.

normalizable and far from the potential

$$\psi(x) \sim e^{-\lambda|x|} \text{ as } |x| \to \infty$$

In particular, bound states is $E < 0$, where $E = -\frac{\hbar^2\lambda^2}{2m}$ which ensures that the particle is trapped within the potential and cannot escape to infinity.

In the other hand, scattering states are not localized in space and, relatedly, the wave functions are not normalizable. Instead, asymptotically, far from the potential, scattering states take the form of plane waves. In one dimension, there are two possibilities

$$\psi \sim e^{ikr} \quad \text{Right moving}$$

$$\psi \sim e^{-ikr} \quad \text{Light moving}$$

Scattering states have $E > 0$. We expect to find solutions for any choice of k.

Reflection and transmission amplitudes

. Suppose that we are so far from the potential and throw particles in, from the left or from the right.

1. Suppose we throw the particle in from the left, this means that we are looking for a solution which asymptotically takes the form

$$\psi_{right}(x) \sim \begin{cases} c^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to +\infty \end{cases}$$

the state ψ_{right} represent the ingoing wave from righ. e^{ikx} represents the particle that we are throwing in from $x \to \infty, re^{-ikx}$ represents the particle that is reflected back to $x \to -\infty$ after hitting the potential, and te^{ikx} represents the particle passing through the potential. Where the coefficient $r \in C$ is called the reflection amplitude, and coefficient $t \in C$ is called the transmission coefficient. Mathematically, we have chosen the solution in which this term vanishes.

The probability for reflection R and transmission T are given by the usual quantum mechanics rule:

$$R = |r|^2 \text{ and } T = |t|^2$$

Given a solution $\psi(x)$ to the Schrödinger equation, we can construct a conserved probability current

$$J(x) = -i\frac{\hbar}{2m}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right)$$

which obeys $dJ/dx = 0$. This means that $J(x)$ is constant. Mathematically, this is the statement that the Wronskian is constant for the two solutions to the Schrödinger equation. For our scattering solution ψ_{right}, the probability current as $x \to -\infty$ is given by

$$\begin{aligned} J(x) &= \frac{\hbar k}{2m}\Big((e^{-ikx} - r^*e^{+ikx})(e^{ikx} - re^{-ikx}) + (e^{ikx} - re^{-ikx})(e^{-ikx} - r^*e^{+ikx})\Big) \\ &= \frac{\hbar k}{m}(1 - |r|^2) \quad x \to -\infty \end{aligned}$$

and as $x \to +\infty$ we have

$$J(x) = \frac{\hbar k}{2m}|t|^2 \quad a \to +\infty$$

The two are giving

$$1 - |r|^2 = |t|^2 \to R + T = 1$$

This means the particle can only get reflected or transmitted and the sum of the probabilities to equals one.

2. Suppose we throw the particle in from the right, again this can hit the potential and get back or pass through straight, we are now looking for solutions which take the asymptotic

form

$$\psi_{left}(x) \sim \begin{cases} t'e^{-ikx} & x \to -\infty \\ e^{-ikx} + r'e^{+ikx} & x \to +\infty \end{cases}$$

the state ψ_{left} represents the ingoing wave at $x \to +\infty$, from left. r' and t' will be the reflection and transmission amplitudes.

Here we will show a simple relation between the two solutions ψ_{right} and ψ_{left}. It follows because the potential $V(x)$ is a real function, so if ψ_{right} is a solution then ψ^t_{right} is a solution too. And, by linearity, so is $\psi^*_{right} - r^*\psi_{right}$ are given by

$$\psi^*_{right}(x) - r^*\psi_{right}(x) \sim \begin{cases} (1-|r|^2)e^{-ikx} & x \to -\infty \\ t^*e^{-ikx} + r^*te^{+ikx} & x \to +\infty \end{cases}$$

we divide through by t^* to make the normalization agree. (scattering states are not normalized anyway). Using $1 - |r|^2 = |t|^2$, which there is a solution of the form ψ_{left} with

$$t' = t \quad \text{and} \quad r' = -\frac{r^*t}{t^*}$$

Note that the transmission amplitudes are always the same, but the reflection amplitudes can differ by a phase. Moreover, the reflection probabilities are the same whether we throw the particle from left or right: $R = |r|^2 = |r'|^2$.

2.2.2 Scattering in higher dimensions

In higher dimension, the phenomenology is similar. Consider a plane wave incident on a localized target; see Figure 2.7.

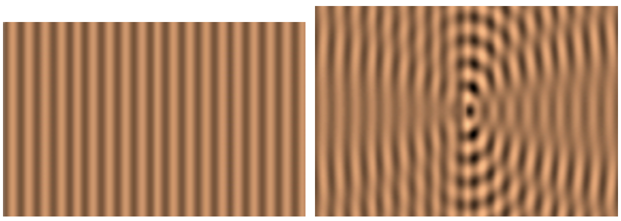

Figure 2.7: Higher dimensional scattering.

Outside localized target region, wavefunction involves superposition of incident plane wave and scattered (spherical wave).

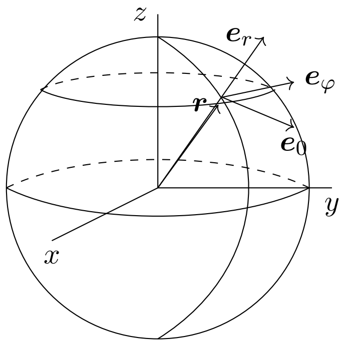

Figure 2.8: Scattered (spherical) wave.

2.2.3 Partial waves

If we define z-axis by $\boldsymbol{k}$ vector, plane wave can be decomposed into superposition of incoming and outgoing spherical wave:

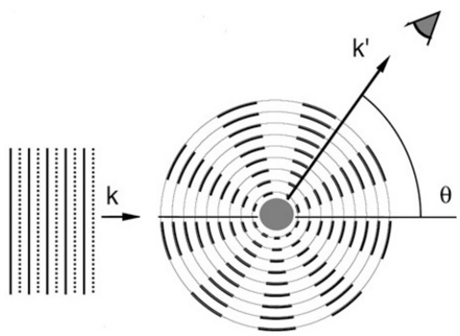

Figure 2.9: Partial wave scattering

If $V(r)$ isotropic, short-ranged (faster than $1/r$), and elastic (particle/energy conserving), scattering wavefunction given by

$$\psi(\boldsymbol{r}) \backsimeq \frac{i}{2k}\sum_{l=0}^{\infty} i^l(2l+1)\left[\frac{e^{-i(kr-l\pi/2)}}{r} - S_l(k)\frac{e^{i(kr-l\pi/2)}}{r}\right]P_l(\cos\theta).$$

If we set, $\psi(\boldsymbol{r}) \backsimeq e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta)\frac{e^{ikr}}{r}$

$$f(\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta).$$

where $f_l(k) = \dfrac{S_l(k)-1}{2ik}$ define partial wave scattering amplitudes, i.e. $f_l(k)$ are defined by phase shifts, $\delta_l(k)$, where $S_l(k) = e^{2i\delta_l(k)}$. But how are phase shifts related to cross section?

2.2.4 Scattering cross section

Bear in mind the picture in Figure 2.5 and

$$\psi(\boldsymbol{r}) \backsimeq e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta)\frac{e^{ikr}}{r}.$$

Let us recall the particle flux associated with $\psi(\boldsymbol{r})$ obtained from the current operator given by

$$\begin{aligned}\boldsymbol{j} &= -i\frac{\hbar}{m}(\psi^*\nabla\psi + \psi\nabla\psi^*) = -i\frac{\hbar}{m}\,\mathrm{Re}\,[\psi^*\nabla\psi] \\ &= -i\frac{\hbar}{m}\,\mathrm{Re}\left\{\left[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta)\frac{e^{ikr}}{r}\right]^*\nabla\left[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta)\frac{e^{ikr}}{r}\right]\right\}\end{aligned}$$

If we neglect rapidly fluctuation contributions (which average to zero) we get

$$\boldsymbol{j} = \frac{\hbar\boldsymbol{k}}{m} + \frac{\hbar k}{m}\hat{e}_r\frac{|f(\theta)|^2}{r^2} + \mathcal{O}(1/r^3)$$

Away from direction of incident beam, $\hat{\boldsymbol{e}}_k$, the flux of particles crossing area, $dA = r^2\,d\Omega$, that subtends solid angle $d\Omega$ at the origin (i.e. the target) given by

$$Nd\Omega = \boldsymbol{j}\cdot\hat{e}_r\,dA = \frac{\hbar K}{m}\frac{|f(\theta)|^2}{r^2}r^2 d\Omega + \mathcal{O}(1/r).$$

By equating this flux with the incoming flux $j_I \times d\sigma$, where $j_I = \dfrac{\hbar k}{m}$, we obtain the differential cross section

$$d\sigma = \frac{Nd\Omega}{j_I} = \frac{\boldsymbol{j}\cdot\hat{e}_r\,dA}{j_I} = |f(\theta)|^2 d\Omega,$$

i.e.,

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2, \qquad \text{where } f(\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta).$$

From the expression for $d\sigma/d\Omega$, we obtain the total scattering cross-section

$$\sigma_{\mathrm{tot}} = \int d\,\mathrm{spec} = \int |f(\theta)|^2\,d\Omega.$$

Applying the orthogonality relation, $\int d\Omega P_l(\cos\theta)P_{l'}(\cos\theta) = \dfrac{4\pi}{2l+1}\delta_{ll'}$, we find that

$$\begin{aligned}\sigma_{\mathrm{tot}} &= \sum_{l,l'}(2l+1)(2l'+1)f_l^*(k)f_{l'}(k)\int d\Omega P_l(\cos\theta)P_{l'}(\cos\theta) \\ &= 4\pi\sum_l(2l+1)|f_l(k)|^2,\end{aligned}$$

where the f_l appear in

$$f(\theta)\sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta).$$

Making use of the relation $f_l(k) = \frac{1}{2ik}(e^{2i\delta_l(k)} - 1) = \frac{e^{i\delta_l(k)}}{k} \sin \delta_l$, we obtain

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l(k).$$

Since $P_l(1) = 1$, $f(0) = \sum_l (2l+1) f_l(k) = \sum_l (2l+1) \frac{e^{i\delta_l(k)}}{k} \sin \delta_l$, we then find

$$\text{Im } f(0) = \frac{k}{4\pi} \sigma_{\text{tot}}.$$

One may show that this "sum rule", known as the Optical Theorem, encapsulates particle conservation.

2.2.5 Method of partial waves in a nutshell

We summarize the method of partial waves, starting from

$$\psi(\boldsymbol{r}) = e^{ik \cdot r} + f(\theta) \frac{e^{ikr}}{r}.$$

The quantum scattering of particles from a localized target is fully characterised by the differential cross section,

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2.$$

The scattering amplitude, $f(\theta)$, which depends on the energy $E = E_k$, can be separated into a set of partial wave amplitudes,

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos \theta),$$

where partial amplitudes, $f_l(k) = \dfrac{e^{i\delta_\ell}}{k} \sin \delta_\ell$ defined by scattering phase shifts $\delta_\ell(k)$. This leads to the question: how are phase shifts determined?

For scattering from a central potential, the scattering amplitude, f , must be symmetrical about axis of incidence; cf. Figure 2.5. In this case, both scattering wavefunction, $\psi(\boldsymbol{r})$, and scattering amplitudes, $f(\theta)$, can be expanded in Legendre polynomials

$$\psi(\boldsymbol{r}) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos \theta).$$

(cf. wavefunction for hydrogen-like atoms with $m = 0$). Each term in the expansion is known as a partial wave, and is simultaneous eigenfunction of $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$ having eigenvalue $\hbar^2 l(l+1)$ and 0, with $l = 0, 1, 2, ...$ referred to as $s, p, d, ...$ waves. From the asymptotic form of $\psi(\boldsymbol{r})$ we can determine the phase shifts $\delta_k(k)$ and in turn the partial amplitudes $f_l(k)$.

$$\psi(\boldsymbol{r}) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos\theta).$$

Starting with Schrödinger equation for scattering wavefunction

$$\left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V(r)\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}), \qquad \text{with } E = \frac{\hbar^2 k^2}{2m}.$$

Then separability of $\psi(\boldsymbol{r})$ leads to the radial equation

$$\left[-\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{2}{r}\partial_r - \frac{l(l+1)}{r^2}\right) + V(r)\right] R_l(r) = \frac{\hbar^2 k^2}{2m} R_l(r).$$

By rearranging this equation, we obtain

$$\left[\partial_r^2 + \frac{2}{r}\partial_r - \frac{l(l+1)}{r^2} - U(r) + k^2\right] R_l(r) = 0,$$

where $U(r) = 2mV(r)/\hbar^2$ represents the effective potential. If we assume that the potential is sufficiently short-ranged, scattering wavefunction involves superposition of incoming and outgoing spherical waves

$$R_l(r) \simeq \frac{i}{2k}\sum_{l=0}^{\infty} i^l (2l+1)\left(\frac{e^{-i(kr - l\pi/2)}}{r} - e^{2i\delta_\ell(k)}\frac{e^{i(kr-l\pi/2)}}{r}\right).$$

$$R_0(r) \simeq \frac{1}{kr} e^{i\delta_0(k)} \sin(kr + \delta_0(k)).$$

However, at low energy, $kR \ll 1$, where R is typical the range of the potential, the s-wave channel ($l = 0$) dominates. Here, with $u(r) = rR_0(r)$, the radial equation becomes

$$[\partial_r^2 - U(r) + k^2]u(r) = 0$$

with boundary condition $u(0) = 0$ and, as expected, outside radius.

Apart from the phase shift, δ_0, it is convenient to introduce scattering length, a_0, defined by the condition that $u(a_0) = 0$ for $kR \ll 1$, i.e.

$$\begin{aligned} u(a_0) &= \sin(ka_0 + \delta_0) = \sin(ka_0)\cos\delta_0 + \cos(ka_0)\sin\delta_0 \\ &= \sin\delta_0[\cot\delta_0 \sin(ka_0) + \cos(kr)] \simeq \sin\delta_0[ka_0\cot\delta_0 + 1] \end{aligned}$$

leads to scattering length $a_0 = -\lim_{k\to 0}(1/k)\tan\delta_0(k)$. From this result, we find the scattering cross section

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sin^2\delta_0(k) \overset{k\to 0}{\simeq} \frac{4\pi}{k^2}\frac{(ka_0)^2}{1+(ka_0)^2} \simeq 4\pi a_0^2.$$

i.e., a_0 characterizes the effective size of target.

2.2.6 Scattering by hard-sphere

We consider hard sphere potential,

$$U(r) = \begin{cases} \infty & r < R \\ 0 & r > R \end{cases}$$

With the boundary condition $u(R) = 0$, suitable for an impenetrable sphere, the scattering wave function is given by

$$u(r) = A\sin(kr + \delta_0), \qquad \delta_0 = -kR.$$

i.e., the scattering length equals $a_0 \backsimeq R$, $f_0(k) = \dfrac{e^{ikR}}{k}\sin(kR)$, and the total scattering cross section is given by

$$\sigma_{\text{tot}} \simeq 4\pi\frac{\sin^2(kR)}{K^2} \simeq 4\pi R^2.$$

The factor of 4 is an enhancement over the classical value, πR^2, and this is due to diffraction processes at sharp potential.

2.2.7 Scattering by attractive square well

As a proxy for scattering from a binding potential, let us consider quantum particles incident upon an attractive square well potential, $U(r) = -U_0\theta(R - r)$, where $U_0 > 0$.

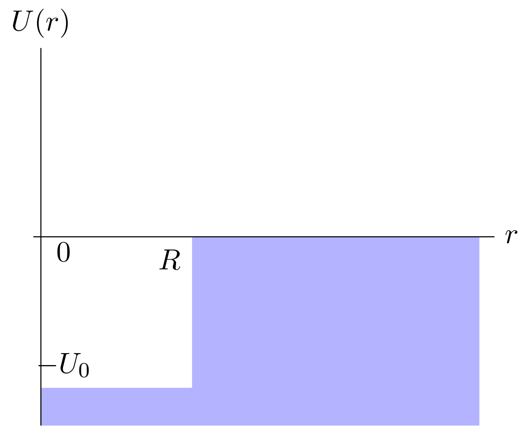

Figure 2.10: Scattering by attractive square well, I.

Once again, focussing on low energies, $kR \ll 1$ this translates to the radial equation

$$[\partial_r^2 - U(0)\theta(R - r) + k^2]u(r) = 0.$$

with the boundary condition $u(0) = 0$. We obtain the solution,

$$u(r) = \begin{cases} C\sin(Kr) & r < R, \\ \sin(kr + \delta_0) & r > R, \end{cases}$$

where $K^2 = k^2 + U_0 > k^2$ and δ_0 denotes scattering phase shift. From continuity of wave function and derivative at $r = R$,

$$C\sin(KR) = \sin(kR + \delta_0), \qquad CK\cos(KR) = k\cos(kR + \delta_0)$$

we obtain the self-consistency condition for $\delta_0 = \delta_0(k)$, namely

$$K\cot(KR) = k\cot(kR + \delta_0).$$

From this result, we obtain

$$\tan\delta_0(k) = \frac{k\tan(KR) - K\tan(kR)}{K + k\tan(kR) - K\tan(KR)}, \qquad K^2 = k^2 + U_0.$$

With $kR \ll 1$, $K \simeq U_0^{1/2}(1 + O(K^2/U_0))$, we find the scattering length

$$a_0 = -\lim_{k\to 0}\frac{1}{k}\tan\delta_0 \simeq -R\left(\frac{\tan(KR)}{KR} - 1\right),$$

which, for $KR < \pi/2$ leads to a negative scattering length. Hence, at low energies, the scattering from an attractive square potential leads to the $l = 0$ phase shift,

$$\delta_0 \simeq -ka_0 \simeq kR\left(\frac{\tan(KR)}{KR} - 1\right)$$

and total scattering cross-section

$$\sigma_{\text{tot}} \simeq \frac{4\pi}{k^2}\sin^2\delta_0(k) \simeq 4\pi R^2\left(\frac{\tan(KR)}{KR} - 1\right)^2, \qquad k \simeq U_0^{1/2}.$$

So, the question arises: what happens when $KR \simeq \pi/2$? If $KR \ll 1$, $a_0 < 0$ and wave function drawn towards target – main characteristic of an attractive potential; see Figure 2.11.

As $KR \to \pi/2$, both scattering length a_0 and cross section $\sigma_{tot} \simeq 4\pi a_0^2$ diverge; see Figure 2.12.

As KR increased, a_0 turns positive, wave function pushed away from target (cf. repulsive potential) until $KR = \pi$ when $\sigma_{\text{tot}} = 0$ and process repeats; see Figure 2.13.

It turns out that when $KR = \pi/2$, the attractive square well just meets the criterion to host a single s-wave bound state. At this value, there is a zero energy resonance leading to the divergence of the scattering length, and with it, the cross section – the influence of the target becomes effectively infinite in range. When $KR = 3\pi/2$, the potential becomes capable of hosting a second bound state, and there is another resonance, and so on.

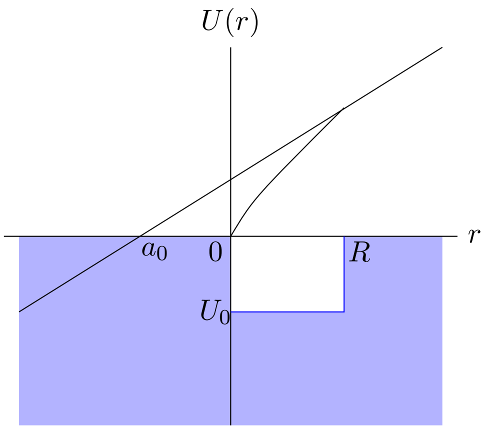

Figure 2.11: Scattering by attractive square well, II.

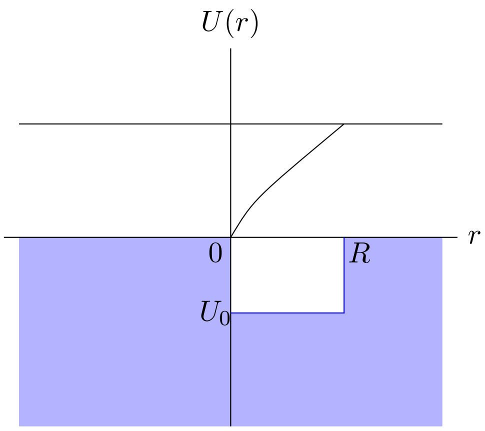

Figure 2.12: Scattering by attractive square well, III.

2.3 Lippmann-Schwinger equation

Returning to Schrödinger equation for scattering wavefunction,

$$(\nabla^2 + k^2)\psi(\boldsymbol{r}) = U(\boldsymbol{r})\psi(\boldsymbol{r})$$

with $V(\boldsymbol{r}) = \dfrac{\hbar^2 U(\boldsymbol{r})}{2m}$, general solution can be written as

$$\psi(\boldsymbol{r}) = \phi(\boldsymbol{r}) + \int G_0(\boldsymbol{r}, \boldsymbol{r}')U(\boldsymbol{r}')\psi(\boldsymbol{r}')\, d^3r'$$

where $(\nabla^2 + k^2)\phi(\boldsymbol{r}) = 0$ and $(\nabla^2 + k^2)G_0(\boldsymbol{r}, \boldsymbol{r}') = \delta^d(\boldsymbol{r} - \boldsymbol{r}')$. Formally, these equations have the solution

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \qquad G_0(\boldsymbol{r}', \boldsymbol{r}') = -\frac{1}{4\pi}\frac{e^{ik|\boldsymbol{r} - \boldsymbol{r}'|}}{|\boldsymbol{r} - \boldsymbol{r}'|}.$$

Together, leads to Lippmann-Schwinger equation

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} - \frac{1}{4\pi}\int d^3r' \frac{e^{ik|\boldsymbol{r} - \boldsymbol{r}'|}}{|\boldsymbol{r} - \boldsymbol{r}'|}U(\boldsymbol{r}')\psi_{\boldsymbol{k}}(\boldsymbol{r}').$$

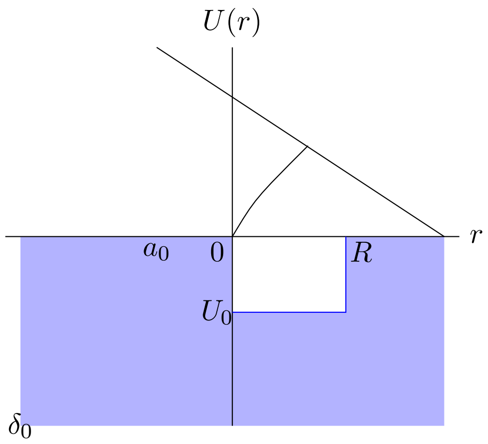

Figure 2.13: Scattering by attractive square well, IV.

In far-field (please see Fig. 2.9), $|\boldsymbol{r}-\boldsymbol{r'}| \backsimeq \boldsymbol{r} - \hat{e_r}\cdot\boldsymbol{r'} + \cdots$,

$$\frac{e^{ik|\boldsymbol{r}-\boldsymbol{r'}|}}{|\boldsymbol{r}-\boldsymbol{r}|} \backsimeq \frac{e^{ikr}}{r} e^{i\boldsymbol{k'}\cdot\boldsymbol{r'}},$$

where $\boldsymbol{k'} \equiv k\hat{e}_r$, i.e. $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta,\phi)\dfrac{e^{ikr}}{r}$ where, with $\phi_{\boldsymbol{k}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$,

$$f(\theta,\phi) \backsimeq -\frac{1}{4\pi}\int d^3r' e^{-i\boldsymbol{k'}\cdot\boldsymbol{r'}} U(\boldsymbol{r'})\psi_{\boldsymbol{k}}(\boldsymbol{r'}) \equiv -\frac{1}{4\pi}\langle\phi_{\boldsymbol{k'}}|U|\psi_{\boldsymbol{k}}\rangle.$$

The corresponding differential cross-section:

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 = \frac{m^2}{(2\pi)^2\hbar^4}|T_{\boldsymbol{k},\boldsymbol{k'}}|^2,$$

where, in terms of the original scattering potential, $V(\boldsymbol{r}) = \dfrac{\hbar^2 U(\boldsymbol{r})}{2m}$,

$$T_{\boldsymbol{k},\,\boldsymbol{k'}} = \langle\phi_{\boldsymbol{k'}}|V|\psi_{\boldsymbol{k}}\rangle$$

denotes the transition matrix element.

2.4 Born approximation

$$\psi(\boldsymbol{r'}) = \phi(\boldsymbol{r'}) + \int G_0(\boldsymbol{r},\boldsymbol{r'})U(\boldsymbol{r'})\psi(\boldsymbol{r'})\, d^3r' \qquad (*)$$

At zeroth order in $V(r)$, scattering wavefunction translates to unperturbed incident plane wave, $\psi^{(0)}_{\boldsymbol{k}}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$. In this approximation, $(*)$ leads to expansion first order in U,

$$\psi^{(1)}_{\boldsymbol{k}}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}(\boldsymbol{r}) + \int d^3r'\, G_0(\boldsymbol{r},\boldsymbol{r'})U(\boldsymbol{r'})\psi^{(0)}_{\boldsymbol{k}}(\boldsymbol{r'})$$

and then to second order in U,

$$\psi_{\boldsymbol{k}}^{(2)}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}(\boldsymbol{r}) + \int d^3r'\, G_0(\boldsymbol{r},\boldsymbol{r}')U(\boldsymbol{r}')\psi_{\boldsymbol{k}}^{(1)}(\boldsymbol{r}')$$

and so on, i.e., expressed in coordinate-independent basis,

$$|\psi_{\boldsymbol{k}}\rangle = |\phi_{\boldsymbol{k}}\rangle + \hat{G}_0\hat{U}\,|\phi_{\boldsymbol{k}}\rangle + \hat{G}_0\hat{U}\hat{G}_0\,|\phi_{\boldsymbol{k}}\rangle + \cdots = \sum_{n=0}^{\infty}(\hat{G}_0\hat{U})^n\,|\phi_{\boldsymbol{k}}\rangle.$$

Then, making use of the identity $f(\theta,\phi) = -\frac{1}{4\pi}\langle\phi_{\boldsymbol{k'}}|U|\psi_{\boldsymbol{k}}\rangle$, scattering amplitude expressed as Born series expansion

$$f = -\frac{1}{4\pi}\langle\phi_{\boldsymbol{k'}}|\,U + UG_0U + UG_0UG_0U + \cdots\,|\phi_{\boldsymbol{k}}\rangle.$$

Physically, incoming particle undergoes a sequence of multiple scattering events from the potential. Leading term in Born series known as first Born approximation (please see Fig. 2.9)

$$f_{Born} = -\frac{1}{4\pi}\langle\phi_{\boldsymbol{k'}}|U|\phi_{\boldsymbol{k}}\rangle.$$

Setting $\Delta = \boldsymbol{K} - \boldsymbol{K}'$, where $\hbar\Delta$ denotes momentum transfer, Born scattering amplitude for a central potential

$$f_{Born}(\Delta) = -\frac{1}{4\pi}\int d^3r e^{i\boldsymbol{\Delta}\cdot\boldsymbol{r}}U(\boldsymbol{r}) = -\int_0^{\infty} r dr \frac{\sin(\Delta r)}{\Delta}U(r),$$

where, noting that $|\boldsymbol{k}'| = |\boldsymbol{k}|, \Delta = 2k\sin(\theta/2)$.

2.5 Coulomb scattering

Because the nucleus has a distribution of electric charge, it can be studied by the electric (Coulomb) scattering of a beam of charged particles. This scattering may be either elastic or inelastic.

Elastic Coulomb scattering is called Rutherford scattering because early (1911-1913) experiments on the scattering of a particles in Rutherford's laboratory by Geiger and Marsden led originally to the discovery of the existence of the nucleus as we discussed in the beginning. The basic geometry for the scattering as is always the case for unbound orbits in a $1/r^2$ force, the scattered particle follows a hyperbolic path.

The case of Coulomb potential is somewhat special because the potential turn off at infinity rather slowly. This asymptotic behaviour, however, is not valid for the Coulomb potential. Coulomb potential is long-ranged and distorts the wave function even at large distances. One finds that the scattering cross section is

$$\frac{d\sigma}{d\O} = |f(\theta)|^2 = \frac{\gamma^2}{4k^2 \sin^4 \theta/2} = \left(\frac{ZZ'e^2}{4E}t\right)^2 \frac{1}{\sin^4 \theta/2}.$$

Due to long range nature of the Coulomb scattering potential, the boundary condition on the scattering wavefunction does not apply. We can, however, address the problem by working with the screened (Yukawa) potential, $U(r) = U_0 \frac{e^{-r/\alpha}}{r}$ and taking $\alpha \to \infty$. For this potential, one may show that

$$f_{\text{Born}} = -U_0 \int_0^\infty dr \frac{\sin(\Delta r)}{\Delta} e^{-r/\alpha} = -\frac{U_0}{\alpha^{-2} + \Delta^2}$$

Therefore, for $\alpha \to \infty$ we obtain

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{U_0^2}{16k^4 \sin^4 \theta/2},$$

which is just the Rutherford formula above.

Notes on bibliography

We have used a number of references to write this chapter. We list them in alphabetical order: [5, 6, 12, 14, 16, 20, 21, 23, 29].

Chapter 3

Linear operators

3.1 Linear operators on Hilbert spaces

Let $\mathcal{H}$ be a complex Hilbert space, i.e.,

Definition 3.1.1 *A Hilbert space $\mathcal{H}$ is a complex vector space, with a scalar (or inner) product $\langle \cdot, \cdot \rangle$, which is complete with respect to the induced norm $\|f\| = \langle f, f \rangle^{1/2}$.*

Let $D \subset \mathcal{H}$ be a linear subset, and let $T : D \to \mathcal{H}$ be a linear (not necessarily continuous) map. For brevity, T is said to be a linear operator in $\mathcal{H}$. The set D is denoted by $\mathrm{Dom}\,(T)$ and called the domain of the operator. If T_1 and T_2 are two linear operators on $\mathcal{H}$, T_2 is said to be an extension of T_1, in symbols, $T_1 \subset T_2$ provided $\mathrm{Dom}\,(T_1) \subset \mathrm{Dom}\,(T_2)$ and $T_1 = T_2$ on $\mathrm{Dom}\,(T_1)$.

Definition 3.1.2 *A map $T : \mathcal{H} \to \mathcal{H}$ is a bounded linear map if T is linear, i.e.,*

$$T(\alpha f + \beta g) = \alpha T f + \beta T g \qquad \text{for all } f, g \in \mathcal{H} \text{ and all } \alpha, \beta.$$

and there exists $C > 0$ such that

$$\|Tf\| \leq C\|f\|, \qquad \forall f \in \mathcal{H}.$$

If $\mathrm{Dom}\,(T) = \mathcal{H}$ and T is bounded, then we write $T \in \mathcal{B}(\mathcal{H})$. We recall three topologies on $\mathcal{B}(\mathcal{H})$. Consider $(T_n)_{n\in\mathbb{N}} \subset \mathcal{B}(\mathcal{H})$.

- (T_n) converges uniformly to $T_\infty \in \mathcal{B}(\mathcal{H})$ if $\|T_n - T_\infty\| \overset{n\to\infty}{\longrightarrow} 0$. We write u $-$ $\lim_{n\to\infty} T_n = T_\infty$.
- (T_n) converges strongly to $T_\infty \in \mathcal{B}(\mathcal{H})$ if $\|(T_n - T_\infty)f\| \overset{n\to\infty}{\longrightarrow} 0$ for $\forall f \in \mathcal{H}$. We write s-$\lim_{n\to\infty} T_n = T$.
- (T_n) converges weakly to T_∞ if $|\langle g, (T_n - T_\infty)f\rangle| \overset{n\to\infty}{\longrightarrow} 0$ for $\forall f, g \in \mathcal{H}$. We write w-$\lim_{n\to\infty} T_n = T_\infty$

If D_0 is a linear subset of D, then $T_0 = T|_{D_0}$ (the notation $T \restriction D_0$ is also used) is said to be a restriction of T. We shall write $T_0 \subset T$. We recall that a subset $D \subset \mathcal{H}$ is called fundamental if finite linear combinations of the vectors in D form a dense subspace of $\mathcal{H}$.

On Dom (T) one can define the graph norm or T-norm $\|\cdot\|_T$ by

$$\|u\|_T^2 = \|Tu\|^2 + \|u\|^2, \quad u \in \mathrm{Dom}\,(T) \tag{3.1}$$

T is said to be a closed operator if Dom (T) is complete in the T-norm. An equivalent definition is this: T is closed if its graph $\mathcal{G}(T) = \{\{u, v\} \in \mathcal{H} \oplus \mathcal{H} : u \in \mathrm{Dom}\,(T), v = Tu\}$ is closed in $\mathcal{H} \oplus \mathcal{H}$. We say that T is a closable operator if the closure of the graph of T in $\mathcal{H} \oplus \mathcal{H}$ is also the graph of an operator. If T is closable, then the operator $\overline{T}$ defined by $\mathcal{G}(\bar{T}) = \overline{\mathcal{G}(T)}$ is called the closure of T; equivalently, T is closable if it has a closed extension $\widetilde{T}$. In this case there is a closed extension $\bar{T}$, which we call its *closure*, whose domain is smallest among all closed extensions. An equivalent condition is that if $(u_n)_n$, where $u_n \in \mathrm{Dom}\,(T)$, is a Cauchy sequence in the T-norm and $\|u_n\| \to 0$, then $\|u_n\|_T \to 0$. The latter property means that the topologies generated by the norm of $\mathcal{H}$ and by the T-norm on Dom (T) are compatible. A core of a closable operator is a subset $\mathfrak{D}$ of Dom (T) such that the closure of the restriction of T to $\mathfrak{D}$ is $\bar{T}$. If T is bounded, then $\bar{T}$ coincides with the extension of T by continuity.

3.2 The adjoint operator

Let T be a densely defined operator, i.e., $\overline{\mathrm{Dom}\,(T)} = \mathcal{H}$.

Definition 3.2.1 (The adjoint operator) *The domain of T^* is*

$$\mathrm{Dom}\,(T^*) := \{v \in \mathcal{H} : \exists\, h \in \mathcal{H} \quad \langle Tu, v\rangle = \langle u, h\rangle \quad \forall u \in \mathrm{Dom}\,(T)\}.$$

The vector h is uniquely determined by v, and we set $h = T^*v$. Thus

$$\langle Tu, v\rangle = \langle u, T^*v\rangle, \qquad \forall u \in \mathrm{Dom}\,(T) \quad \forall v \in \mathrm{Dom}\,(T^*).$$

Definition 3.2.2 (self-adjoint operator) *We say that an operator T is self-adjoint if*

$$T^* = T, \ \ i.e.$$

$$Tu = T^*u$$

and that is T is self-adjoint if and only if

$$\langle Tu, v\rangle = \langle u, Tv\rangle \quad \forall\, u, v \in \mathrm{Dom}\,(T)$$

As opposed to the case of $T \in \mathcal{B}(\mathcal{H})$, this equality is used not only to describe the 'action' of T^*, but, as we can see, also to describe the domain of T^*.

The adjoint operator T^* is always a closed operator, $\overline{\mathrm{Dom}\,(T^*)} = \mathcal{H}$ if and only if T is closable. Under this assumption, $(T^*)^* = \overline{T}$. If $T_0 \subset T$ and $\overline{\mathrm{Dom}\,(T_0)} = \mathcal{H}$, then $T_0^* \supset T^*$.

3.3 Self-adjoint operators

We recall the definitions of symmetric and self-adjoint operators.

Definition 3.3.1 *An operator T such that $T^* = T$ is said to be self-adjoint. An operator T such that $\overline{\mathrm{Dom}\,(T)} = \mathcal{H}$ and*

$$\langle Tu, v\rangle = \langle u, Tv\rangle, \quad \forall u, v\, \mathrm{Dom}\,(T),$$

is called symmetric. Those two notions are equivalent for $T \in \mathcal{B}(\mathcal{H})$. If $T^* = \overline{T}$, then T is said to be essentially self-adjoint. If T is symmetric and $\overline{T} = T^*$, the T^* is seen not to be symmetric.

The self-adjointness of an operator can often be established by means of perturbation theory, i.e., from the fact that the operator is close to another operator known in advance to be self-adjoint. The following theorem is a typical result in this direction.

Theorem 3.3.2 *(Kato-Rellich; see Kato 1966; Reed and Simon 1975, Vol.2).*
Let T be a self-adjoint operator and let S be a symmetric operator in Hilbert space $\mathcal{H}$ such that $\mathrm{Dom}\,(S) \supset \mathrm{Dom}\,(T)$ and

$$\|Su\| \leq a\|Tu\| + b\|u\| \quad \forall u \in \mathrm{Dom}\,(T) \tag{3.2}$$

for some $0 < a < 1$ and $b \geq 0$. Then $T + S$ is self-adjoint on $\mathrm{Dom}\,(T)$ and essentially self-adjoint on any domain of essential self-adjointness of T.

Lemma 3.3.3 *If T is self-adjoint and $z \in \mathbb{C}$, then $z \in \rho(T)$ if and only if there exists $c > 0$ such that $\|(T - z)u\| \geq c\|u\|$ for all $u \in \mathrm{Dom}\,(T)$*

Proof. Let $z \in \mathbb{C}$ and assume that $c > 0$ is such that $\|(z - T)u\| \geq c\|u\|$ for all $u \in \mathrm{Dom}\,(T)$. We also have, for all $u \in \mathrm{Dom}\,(T) = \mathrm{Dom}\,(T^*)$, $\|(\bar{z} - T)u\| \geq c\|u\|$. Then $\mathrm{Ker}\,(z - T) = \mathrm{Ker}\,(\bar{z} - T) = \{0\}$ and $\mathrm{Ran}\,(z - T)$ is dense, since if $v \in \mathrm{Ran}\,(z - T)^{\perp}$ then for all $u \in \mathrm{Dom}\,(T), 0 = \langle v, (z - T)u\rangle$, so $v \in \mathrm{Dom}\,(T^*) = \mathrm{Dom}\,(T)$, and $(\bar{z} - T)v = 0$ and hence $v = 0$. It remains to prove that $\mathrm{Ran}\,(z - T) = \mathcal{H}$. We have :

$$\forall u \in \mathrm{Dom}\,(T), \quad \|(z - T)u\|^2 = \|(\mathrm{Re}\ z - T)u\|^2 + (\mathrm{Im}\ z)^2\|u\|^2. \tag{3.3}$$

Then if for all $n \in \mathbb{N}$, $v_n = (z - T)u_n \in \mathrm{Ran}\,(z - T)$ and $v_n \to v$ as $n \to \infty$, by (3.3), $(u_n)_{n\in\mathbb{N}}$ is a Cauchy sequence, and tends to some $u \in \mathcal{H}$, and (Tu_n) converges too. As T is closed, $u \in \mathrm{Dom}\,(T)$ and $v = (z - T)u \in \mathrm{Ran}\,(z - T)$, so $\mathrm{Ran}\,(z - T)$ is closed. Thus $z \in \rho(T)$.

Conversely, we assume that $z \in \rho(T)$. If $z \notin \mathbb{R}$, then we have the result by (3.3). Then suppose $z \in \mathbb{R}$. Let $u \in \mathcal{H} \setminus \{0\}$ and $v = (z - T)^{-1}u$. We have :

$$\|u\|^2 = \langle u, (z - T)v\rangle = \langle (z - T)u, v\rangle \leq \|(z - T)u\|\|(z - T)^{-1}\|\,\|u\|$$

and hence we have $\|(z - T)u\| \geq \|(z - T)^{-1}\|^{-1}\|u\|$. $\square$

3.4 Various operators

We collect the following definitions.

Definition 3.4.1 *Let $T \in \mathcal{B}(\mathcal{H})$.*

- *T is self-adjoint if $T^* = T$*
- *T is normal if $T^*T = TT^*$*
- *T is a projection if $T^2 = TT = T$,*
- *T is an orthogonal projection if $T^2 = T = T^*$,*
- *T is unitary if $TT^* = I$ and $T^*T = I$, where I is the identity operator, i.e. $If = f, \forall f \in \mathcal{H}$.*
- *T is an isometry if $T^*T = I$.*
- *T is a partial isometry if T^*T is an orthogonal projection.*

We also recall the definition of a compact operator.

Definition 3.4.2 *$T \in \mathcal{B}(\mathcal{H})$ is a compact operator if $\exists (T_n) \subset \mathcal{F}(\mathcal{H})$ such that $u - \lim_{n\to\infty} T_n = T$. We set $\mathcal{B}_\infty(\mathcal{H}) = \{$all compact operator$\} \subset \mathcal{B}(\mathcal{H})$.*

Compact operators have the following properties.

- $T \in \mathcal{B}_\infty(\mathcal{H}) \Rightarrow T^* \in \mathcal{B}_\infty(\mathcal{H})$.
- $\mathcal{B}_\infty(\mathcal{H})$ is norm closed.
- If $S \in \mathcal{B}(\mathcal{H}),\ T \in \mathcal{B}_\infty(\mathcal{H}) \Rightarrow ST, TS \in \mathcal{B}_\infty(\mathcal{H})$.
- If $f_n \overset{n\to\infty}{\underset{w}{\longrightarrow}} f_\infty$ and $T \in \mathcal{B}_\infty(\mathcal{H})$, then $Tf_n \overset{n\to\infty}{\underset{s}{\longrightarrow}} Tf_\infty$.
- If $S_n \overset{n\to\infty}{\underset{s}{\longrightarrow}} S_\infty$ and $T \in \mathcal{B}_\infty(\mathcal{H})$, $S_nT \overset{n\to\infty}{\underset{u}{\longrightarrow}} S_\infty T$ and $TS_n^* \overset{n\to\infty}{\underset{u}{\longrightarrow}} TS_\infty^*$.

We need the following result in the sequel.

Proposition 3.4.3 *Let $f \in C_\infty(\mathbb{R})$, the continuous function vanishing at infinity, and let A and B be self-adjoint operators such that $(A-z)^{-1} - (B-z)^{-1}$ is compact for all non-real z, then $f(A) - f(B)$ is compact.*

Proof. According to the Stone-Weierstrass Theorem [28, Theorem IV.9], polynomials in $(x+i)^{-1}$ and $(x-i)^{-1}$ are dense in $C_\infty(\mathbb{R})$, so by norm closure of the compact operators, it suffices to show that $P_{n,m}(A) - P_{n,m}(B)$ is compact, where n, m are positive integer and $P_{n,m}(x) = (x+i)^{-n}(x-i)^{-m}$ to do this. Let $\phi_{z,w}(x)$ be the function $(w-z)^{-1}[(x-z)^{-1} - (x-w)^{-1}]$. If we can show that $\phi_{z,w}(A) - \phi_{z,w}(B)$ is compact, the Cauchy integral formula gives us that the operators $(\partial/\partial z)^n(\partial\backslash\partial w)^m(\phi_{z,w}(A) - \phi_{z,w}(B))$ are compact. Since $P_{n,m}(x) = (\partial/\partial z)^n(\partial/\partial w)^m|_{-z\,o\,w=i\phi_{z,w}(x)}$ it follows that $P_{n,m}(A) - P_{n,m}(B)$ is compact for each n, m and, by hypothesis,

$$\phi_{z,w}(A) - \phi_{z,w}(B) = (w-z)^{-1}\left\{[(A-z)^{-1} - (B-z)^{-1}] - [(A-w)^{-1} - (B-w)^{-1}]\right\}$$

is compact. □

3.5 Spectrum of an operator

Let $(T, \mathrm{Dom}\,(T))$ be a closed operator on a complex Hilbert space $\mathcal{H}$. A scalar λ is said to be an eigenvalue of T if there exists a non-zero $u \in \mathrm{Dom}\,(T)$ such that $Tu = \lambda u$. The vector u is called an eigenvector (or eigenfunction if $\mathcal{H}$ is a function space) of the operator T. The resolvent set $\rho(T)$ of T is the set defined by

$$\rho(T) = \{\lambda \in \mathbb{C} : T - \lambda I \text{ is one to one and } (T-\lambda I)^{-1} : \mathcal{H} \to \mathcal{H} \text{ is bounded}\}$$

(I being the identity operator in $\mathcal{H}$) and, for $\lambda \in \rho(T)$, the operator $(T-\lambda)^{-1}$ is called the resolvent of T. The complement $\mathrm{spec}\,(T) = \mathbb{C} \setminus \rho(T)$ of the resolvent set is called the spectrum of T. The set $\rho(T)$ is open and $\mathrm{spec}\,(T)$ is closed. It is possible that $\rho(T) = \mathbb{C}$ or $\mathrm{spec}\,(T) = \emptyset$. (For $T \in \mathcal{B}(\mathcal{H})$ neither of those possibilities can be realized).

If $T = T^*$, then the spectrum of T is non-empty and lies on the real axis. The spectrum $\mathrm{spec}\,(T)$ of a self-adjoint operator can be represented as the union of the point spectrum $\mathrm{spec}_\mathrm{p}\,(T)$ (i.e., the set of all eigenvalues) and the continuous spectrum

$$\mathrm{spec}_\mathrm{c}\,(T) = \{\lambda \in \mathbb{R} : \mathrm{Im}\,(T-\lambda I) \text{ is a non-closed set}\}.$$

The spectra $\mathrm{spec_p}(T)$ and $\mathrm{spec_c}(T)$ can have a non-empty intersection. If $\mathrm{spec_p}(T) = \emptyset$, then T has a purely continuous spectrum. If the linear hull of the eigenspaces $\mathrm{Ker}\,(T - \lambda I)$, where $\lambda \in \mathrm{spec_p}(T)$, is dense in $\mathcal{H}$, then T has a pure point spectrum. In this case the continuous spectrum coincides with the set of limit points of the point spectrum and , generally speaking, is non-empty.

The union of the continuous spectrum and the set of eigenvalues of infinite multiplicity is called the essential spectrum of a self-adjoint operator T, denoted by $\mathrm{spec_{ess}}(T)$. If $\mathrm{spec_{ess}}(T) = \emptyset$, then T is an operator with discrete spectrum. An equivalent condition for T to have discrete spectrum is that $(T - \lambda I)^{-1}$ be a compact operator for some $\lambda \in \rho(T)$ (and then for all such λ).

In the sequel we need the following general result on the essential spectrum.

Proposition 3.5.1 *Let T be a self-adjoint operator. An open set $\Omega \subset \mathbb{R}$ is disjoint from* $\mathrm{spec_{ess}}(T)$ *if and only if $f(T)$ is compact for every continuous function f which is compactly supported in Ω.*

Proof. If $\Omega \cap \mathrm{spec_{ess}}(T) = \emptyset$, then $E_K(T)$ has finite dimensional range for any compact $K \subset \Omega$. Let $f \in C(R)$ have compact support $K \subset \Omega$. Then $E_K(T)f(T) = f(T)E_K(T)$ which shows that $f(T)$ has finite rank. Assume, conversely, that every such $f(T)$ is compact. Then, for any $\lambda \in \Omega$, we can pick an f with compact support contained in Ω and $f = 1$ near λ. Since $f(T)$ is compact, we infer that for $\epsilon > 0$ sufficiently small, the projection $E_{\lambda-\epsilon,\lambda+\epsilon}(T) = f(T)E_{\lambda-\epsilon,\lambda+\epsilon}(T)$ is compact and, consequently, finite-dimensional. In conclusion, $\Omega \cap \mathrm{spec_{ess}}(T) = \emptyset$. □

3.6 Spectral Theorem for a self-adjoint operator

The Spectral Theorem is a collection of results which, basically, provide conditions under which a linear operator can be diagonalized. In finite dimension, it states that an operator is self-adjoint if and only if the spectrum is a subset of the real axis and there exists an orthonormal basis consiting of eigenvectors. But in general, when the concept of diagonalization is not straightforward, the Spectral Theorem identifies the operators that can be viewed as multiplication operators, which are as simple as we can hope. It can be stated as follows :

Theorem 3.6.1 (Spectral Theorem - Multiplication operator form) *Let T be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ with domain* $\mathrm{Dom}\,(T)$*. Then there exist a measure space (M, μ) with μ a finite measure, a unitary operator $U : \mathcal{H} \to L^2(M, d\mu)$, and a real-valued function f on M which is finite a.e. so that :*

(a) $\psi \in \mathrm{Dom}\,(T)$ if and only if $f(\cdot)(U\psi)(\cdot) \in L^2(M, d\mu)$.

(b) If $\phi \in U(\mathrm{Dom}\,(T))$, then $(UTU^{-1}\phi)(x) = f(x)\phi(x)$.

Another version of the theorem can be reached as follows. Suppose that associated with every Borel set $\Omega \subset \mathbb{R}$ is an orthogonal projection $E(\Omega)$ in $\mathcal{H}$. Let $E(\mathbb{R}) = I$ and let the following condition of countable additivity be satisfied: if $\{\Omega_n\}, n = 1, 2, \cdots$ are pairwise disjoint Borel sets, then $\sum_n E(\Omega_n) = E(\bigcup_n \Omega_n)$. (The series on the left-hand side converges in the strong operator topology). Any such map $E : \Omega \to E(\Omega)$ is called a spectral measure in $\mathcal{H}$ (defined on the Borel subsets of the real axis).

If E is a spectral measure, then, for any $u \in \mathcal{H}, E(\cdot)u$ is a vector-valued measure and $\mu_u(\cdot) = \langle E(\cdot)u, u\rangle$ is a scalar-valued Borel measure normalized by $\mu_u(\mathbb{R}) = \|u\|^2$. For any $u, v \in \mathcal{H}, \mu_{u,v}(\cdot) = \langle E(\cdot)u, v\rangle$ is a complex-valued Borel measure.

As in the case of scalar measures, the support of a spectral measure (supp E) can be defined as the smallest closed subset $F \subset \mathbb{R}$ such that $E(F) = I$. The expression 'almost everywhere with respect to E' (E-a.e.) has the standard meaning.

Let E a spectral measure and let φ be a Borel measurable scalar function defined E-a.e. on $\mathbb{R}$. Then one can define the integral

$$J_\varphi = \int \varphi dE \qquad \left(= \int \varphi(s) dE(s) \right), \tag{3.4}$$

which is a closed operator in $\mathcal{H}$ with dense domain

$$D(J_\varphi) = D_\varphi = \left\{ u \in \mathcal{H} : \int |\varphi|^2 d\mu_u < \infty \right\}. \tag{3.5}$$

The integral (3.4) can be understood, for example, in the 'weak sense,' that is, $(J_\varphi u, y) = \int \varphi d\mu_{u,y}$ for $u \in D_\varphi$ and $y \in \mathcal{H}$. The operator J_φ is bounded if and only if φ is E-a.e. bounded.

Then the spectral theorem takes the form:

Theorem 3.6.2 *To every self-adjoint operator T there corresponds a unique spectral measure E_T such that*

$$T = \int s \, dE_T(s). \tag{3.6}$$

It turns out that $\operatorname{supp} E_T = \operatorname{spec}(T)$.

The relation

$$u = \int dE_T(s)u, \qquad \|u\|^2 = \int d\mu_u^T(s) \qquad \forall u \in \mathcal{H}, \tag{3.7}$$

$$\operatorname{Dom}(T) = \left\{ u \in \mathcal{H} : \int s^2 d\mu_u^T(s) < \infty \right\}, \tag{3.8}$$

where $\mu_u^T(\cdot) = (E_T(\cdot)u, u)$, follow from Theorem 3.6.2 together with (3.5). They express the decomposition theorem.

The operators $J_\varphi^T = \int \varphi dE_T$ can be regarded as function $\varphi(T)$ of a self-adjoint operator T, which is consistent with the direct definition of the powers T^n (for $\varphi(s) = s^n$) and the resolvent $(T - \lambda I)^{-1}$ for $\lambda \notin \operatorname{spec}_\mathrm{p}(T)$ (in which case $\varphi(s) = (s-\lambda)^{-1}$)

Example 3.6.3. Let T be a self-adjoint operator with pure point spectrum and let $P(\lambda)$, where $\lambda \in \operatorname{spec}_\mathrm{p}(T)$, be the orthogonal projections onto the eigenspaces $\operatorname{Ker}(T - \lambda I)$. Then the spectral measure E_T can be defined by

$$E_T(\Omega) = \sum_{\lambda \in \Omega} P(\lambda)$$

and the decomposition theorem, see (3.7), takes the simpler form

$$u = \sum_{\lambda \in \operatorname{spec}_\mathrm{p}(T)} P(\lambda)u, \qquad \|u\|^2 = \sum_{\lambda \in \operatorname{spec}_\mathrm{p}(T)} \|P(\lambda)u\|^2. \tag{3.9}$$

In this case

$$\varphi(T) = \sum_{\lambda \in \operatorname{spec_p}(T)} \varphi(\lambda) P(\lambda). \tag{3.10}$$

If $\{e_n\}_1^\infty$ is a complete orthogonal system of eigenvectors of T, then (3.10) means that the Fourier expansion and the Parseval formula

$$u = \sum_n (u, e_n) e_n, \qquad \|u\|^2 = \sum_n |(u, e_n)|^2$$

are both valid for any $u \in \mathcal{H}$.

Theorem 3.6.4 (Spectral Theorem, Functional calculus form) *There exists a unique linear map $f \to f(T)$ from $C_0(\mathbb{R})$ (the space of continuous complex-valued functions on $\mathbb{R}$, which vanish at $\pm\infty$, with the supremum norm) to $\mathcal{B}(\mathcal{H})$ (bounded operators on $\mathcal{H}$) such that :*

(a) The map $f \to f(T)$ is multiplicative (i.e., is an algebra homomorphism).

(b) $\forall f \in C_0(\mathbb{R}), \bar{f}(T) = f(T)^*$

(c) $\forall f \in C_0(\mathbb{R}), \|f(T)\| \leq \|f\|_\infty$

(d) If $w \notin \mathbb{R}$ and $r_w : s \to (w - s)^{-1}$, then $r_w(T) = (w - T)^{-1}$

(e) If $f \in C_0(\mathbb{R})$ has support disjoint from $\operatorname{spec}(T)$, then $f(T) = 0$.

This theorem can be extended as follows :

Theorem 3.6.5 *There exists a map $f \to f(H)$ from $\mathfrak{B}$ (algebra of bounded Borel measurable functions on $\mathbb{R}$) to $\mathcal{B}(\mathcal{H})$ which extends the map of theorem 3.6.4, and has the same properties with the replacement of $C_0(\mathbb{R})$ by $\mathfrak{B}$. The extension is unique subject to the further requirement that $\operatorname{s-lim}_{n\to\infty} f_n(T) = f(T)$ whenever $f_n \in \mathfrak{B}$ converges monotonically to $f \in \mathfrak{B}$.*

Using this last theorem, we see that taking $\chi_B(T)$ for all Borel sets B of the real line and χ_B the characteristic function of B, we get a projection-valued measure, which we denote by $E_T(B) = \chi_B(T)$. Hence $E_T(\cdot)$ is a projection-valued function defined for all Borel sets of the real line with the following properties :

$$E_T(S \cap S') = E_T(S)E_T(S') \tag{3.11}$$

$$E_T\left(\bigcup_{n=0}^{\infty} S_n\right) = \sum_{n=0}^{\infty} E_T(S_n) \text{ for pairwise disjoint } S_n, n \in \mathbb{N} \tag{3.12}$$

But we can also start from this spectral family and write a self-adjoint operator according to its spectral representation :

Theorem 3.6.6 (Spectral Theorem - Spectral representation form) *For every self-adjoint operator T, there exists a projection-valued measure E_T such that :*

$$\forall f \in C(\mathbb{R}), \quad f(T) = \int_{\mathbb{R}} f(\lambda)\, dE_T(\lambda) \tag{3.13}$$

where $C(\mathbb{R})$ is the set of complex-valued continuous functions. If f is bounded on the support of E_T, then $f(T)$ is bounded.

An equivalent version of the spectral theorem is :

Theorem 3.6.7 *For every self adjoint operator T on the Hilbert space $\mathcal{H}$ there exists exactly one spectral family E_T for which $T = \int \lambda\, dE_T(\lambda)$. In the complex case the spectral family is given by :*

$$\langle v, (E_T(b) - E_T(a))u\rangle = \lim_{\delta \to 0^+} \lim_{\epsilon \to 0^+} \frac{1}{2\pi i} \int_{a+\delta}^{b+\delta} \langle v, (R(t - i\epsilon, T) - R(t + i\epsilon, T))u\rangle\, dt \tag{3.14}$$

for all $u, v \in \mathcal{H}$ and $-\infty < a \leq b < +\infty$.

We have :

$$\forall u \in \mathrm{Dom}\,(T), \forall v \in \mathcal{H} \quad \langle Tu, v\rangle = \int_{\mathbb{R}} \lambda\, d\langle E_T(\lambda)u, v\rangle \tag{3.15}$$

Proofs and further details about the Spectral Theorem are given in [28] and [18].

3.7 Partial isometries

Definition 3.7.1 *$W \in \mathcal{B}(\mathcal{H})$ is called a* partial isometry*, if there exists a closed subspace M of $\mathcal{H}$ such that $\|W\psi\| = \|\psi\|$ for all $\psi \in M$ and $W\psi = 0$ for all $\psi \in M^{\perp}$.*

Proposition 3.7.2 *Let $W \in \mathcal{B}(\mathcal{H})$. The following assertions are equivalent :*

1. W is a partial isometry with initial subspace M and final subspace N.

2. Ran $(W) = N$ *and $W^*W = P_M$ (P_M denotes the orthogonal projection onto M).*

3. $W^*W = P_M$ and $WW^* = P_N$.

4. W^* is a partial isometry with initial subspace N and final subspace M.

Proof. $1 \Rightarrow 2$: Let $u \in M$. For all $v \in M$, we have $\langle u, v\rangle = \langle Wu, Wv\rangle = \langle W^*Wu, v\rangle$, so $u - W^*W \in M^\perp$, and for all $w \in M^\perp$, $\langle W^*Wu, w\rangle = \langle Wu, Wu\rangle = 0$ since $Wu = 0$, so $W^*Wu \in (M^\perp)^\perp = M$ since M is closed. Hence $u - W^*Wu \in M \cap M^\perp$, and $W^*Wu = u = P_M u$. Let $u \in M^\perp$. $\forall v \in \mathcal{H}, \langle W^*Wu, v\rangle = \langle Wu, Wv\rangle = 0$, so $W^*Wu = 0 = P_M u$. Hence $W^*W = P_M$.

$2 \Rightarrow 3$: Let $u \in N^\perp$. Then $\|W^*u\|^2 = \langle WW^*u, u\rangle = 0$, thus $N^\perp \subset \text{Ker } W^* \subset \text{Ker } WW^*$. Let now $\phi \in N$. There exists $v \in \mathcal{H}, v_M \in M$ and $v_{M^\perp} \in M^\perp$ such that $v = v_M + v_{M^\perp}$ and $\phi = Wv$. Then :

$$WW^*\phi = WW^*Wv = WP_M v = W(v - v_{M^\perp}) = \phi - Wv_{M^\perp}$$

but $\|Wv_{M^\perp}\|^2 = \langle W^*Wv_{M^\perp}, v_{M^\perp}\rangle = 0$ and hence $WW^*\phi = \phi$. We conclude that $WW^* = P_N$.

$3 \Rightarrow 1$: If $\psi \in M$, then $\langle W\psi, W\psi\rangle = \langle \psi, W^*W\psi\rangle = \langle \psi, \psi\rangle$, and if $\psi \in M^\perp$, then $\|W\psi\|^2 = \langle \psi, W^*W\psi\rangle = 0$, so W is a partial isometry with initial subspace M. Let $\phi \in N$. $\phi = WW^*\phi \in \text{Ran } W$. Conversely, if $\psi \in M$, then $W\psi = W(W^*W\psi) = P_N W\psi \in N$, so Ran $W \subset N$. Hence the final subspace of W is N.

As $(W^*)^* = W$, $1 \Leftrightarrow 3$ implies $4 \Leftrightarrow 3$, which concludes the proof. □

3.8 Stone's theorem

We begin with a definition.

Definition 3.8.1 *A family $(U_t)_{t\in\mathbb{R}}$ is a strongly continuous unitary group if*

1) U_t is unitary for any t.

2) $U_tU_s = U_{t+s}, \qquad \forall t, s \in \mathbb{R}$.

3) s-$\lim_{t\to 0} U_t = I$.

One has:

Theorem 3.8.2 (Stone's theorem) *There exists a bijective relation between self-adjoint operators* $(T, \mathrm{Dom}\,(T))$ *and strongly continuous unitary groups.*

Proof and further details about Stone's Theorem is given in [28], page 266, Theorem VIII.8.

Notes on bibliography

We have used a number of references to write this chapter. We list them in alphabetical order: [2, 3, 4, 8, 1, 18, 24, 28, 25, 27].

Chapter 4

Decompositions of the spectrum

We consider a self-adjoint operator T on a Hilbert space $\mathcal{H}$. The resolvent set and the spectrum of T are respectively denoted by $\rho(T)$ and $\operatorname{spec}(T)$.

4.1 Parts of the spectrum

Let $\mathcal{H}$ be a Hilbert space.

Definition 4.1.1 *Let T be an operator in a Hilbert space $\mathcal{H}$ defined on the domain $\operatorname{Dom}(T)$. The operator T is said to commute with a bounded operator $A \in \mathcal{B}(\mathcal{H})$ if $\operatorname{Dom}(T)$ is invariant under A, i.e., $A \operatorname{Dom}(T) \subseteq \operatorname{Dom}(T)$ and*

$$TAu = ATu, \quad \text{for all } u \in \operatorname{Dom}(T).$$

In symbols, $AT \subseteq TA$.

Definition 4.1.2 *Suppose that M and N are subspaces such that $\mathcal{H} = M \oplus N$. It is said that T can be decomposed with respect to M and N if*

$$P_M \operatorname{Dom}(T) \subseteq \operatorname{Dom}(T), \quad TM \subseteq M, \quad TN \subseteq N,$$

where P_M is the projection onto M along N.

If T is a self-adjoint operator, which can be decomposed with respect to the subspaces M

and $M^\perp$, then it is said that M (or $M^\perp$) reduces T. These notions are tied together by the following proposition.

Proposition 4.1.3 *Suppose $\mathcal{H} = M \oplus N$. An operator T, defined on* $\operatorname{Dom}(T)$*, can be decomposed with respect to M and N if and only if*

$$P_M T \subseteq T P_M,$$

where P_M is the projection onto M along N.

Proof. If T can be decomposed with respect to M and N, then $P_M \operatorname{Dom}(T) \subseteq \operatorname{Dom}(T)$ by definition and if $u \in \operatorname{Dom}(T)$ then

$$TP_M u = P_M T P_M u = P_M T(P_M + P_N)u = P_M T u,$$

because $P_M T P_N u = 0$; T leaves N invariant. Hence we infer that P_M and T commute. If $P_M T \subseteq P_M T$, then, by definition, $P_M \operatorname{Dom}(T) \subseteq \operatorname{Dom}(T)$ and if $u \in \operatorname{Dom}(T) \cap M$ we have that

$$Tu = TP_M u = P_M T u \in M.$$

If $u \in \operatorname{Dom}(T) \cap N$, then

$$Tu = T(I - P_M)u = (I - P_M)Tu \in N,$$

which completes the proof. □

If an operator T can be decomposed with respect to the subspaces M and N, then one can define the restrictions of T, denoted T_M and T_N, onto these subspaces by

$$\operatorname{Dom}(T_M) = P_M \operatorname{Dom}(T); \quad T_M u = Tu, \quad u \in \operatorname{Dom}(T_M),$$

and analogously for T_N.

Theorem 4.1.4 *Suppose that T is a self-adjoint operator on $\mathcal{H}$. If T is reduced by a subspace $M \subseteq \mathcal{H}$, then T_M and $T_{M^\perp}$ are self-adjoint operators. Moreover,* $\operatorname{spec}(T) = \operatorname{spec}(T_M) \cup \operatorname{spec}(T_{M^\perp})$.

Proof. The operator T_M is densely defined. Indeed, suppose $u \in M$ and $\epsilon > 0$ is arbitrary. Then we can find $v \in \operatorname{Dom}(T)$ such that $\|u - v\|_{\mathcal{H}} < \epsilon$ because T is densely defined. Since

M reduces T, we have that $v' := P_M v \in \mathrm{Dom}\,(T) \cap M = \mathrm{Dom}\,(T_M)$ and

$$\|u - v'\|_{\mathcal{H}} = \|P_M(u - v)\|_{\mathcal{H}} \leq \|u - v\|_{\mathcal{H}} < \epsilon.$$

It follows from the fundamental criterion for self-adjointness (see, e.g., [28], that T_M is self-adjoint: suppose $u \in \mathrm{Dom}\,((T_M)^*)$ and$((T_M)^* + i)u = 0$. Let $v = v' + v'' \in \mathrm{Dom}\,(T)$, where $v' \in \mathrm{Dom}\,(T_M)$ and $v'' \in \mathrm{Dom}\,(T_{M^\perp})$. Then

$$\begin{aligned} 0 &= \langle ((T_M)^* + i)u, v\rangle_{\mathcal{H}} = \langle ((T_M)^* + i)u, v'\rangle_{\mathcal{H}} \\ &= \langle u, (T_M + i)v')\rangle_{\mathcal{H}} = \langle u, (T + i)v\rangle_{\mathcal{H}}. \end{aligned}$$

Since $\mathrm{Ran}\,(T + i) = \mathcal{H}$, we deduce $u = 0$. The same argument can be applied if $((T_M)^*) - i)u = 0$ so that $\mathrm{Ker}\,((T_M)^* \pm i) = \{0\}$ and T_M is self-adjoint. Let $u = u' + u'' \in \mathrm{Dom}\,(T)$, where $u' \in \mathrm{Dom}\,(T_M)$ and $u'' \in \mathrm{Dom}\,(T_{M^\perp})$. For $\zeta \in \mathbb{C}$ we have that

$$\|(T - \zeta)u\|^2_{\mathcal{H}} = \|(T - \zeta)u'\|^2_{\mathcal{H}} + \|(T - \zeta)u''\|^2_{\mathcal{H}},$$

whence $\rho(T) = \rho(T_M) \cap \rho(T_{M^\perp})$ or, equivalently, $\mathrm{spec}\,(T) = \mathrm{spec}\,(T_M) \cup \mathrm{spec}\,(T_{M^\perp})$. $\square$

Let T be a self-adjoint operator on $\mathcal{H}$. In the sequel $E(\lambda)$, $\lambda \in \mathbb{R}$, will denote the spectral family associated to T. The spectral family defines a spectral measure $E(\Omega)$, where Ω is a Borel set.

Theorem 4.1.5 *A subspace $M \subseteq \mathcal{H}$ reduces T if and only if*

$$E(\lambda)P_M = P_M E(\lambda), \quad \forall \lambda \in \mathbb{R}.$$

Proof. Suppose M reduces T. According to Proposition 4.1.3, we have that $P_M T \subseteq T P_M$. For $\zeta \in \rho(T)$ and $R(\zeta) = (T - \zeta)^{-1}$ one has

$$R(\zeta)P_M = R(\zeta)P_M(T - \zeta)R(\zeta) \subseteq R(\zeta)(T - \zeta)P_M R(\zeta) = P_M R(\zeta).$$

Since $\mathrm{Ran}\ R(\zeta) = \mathrm{Dom}\,(T)$, one has equality and P_M thus commutes with all the resolvents of T. That P_M also commutes with $E(\lambda)$ follows from Stone's formula, see (3.14),

$$\frac{1}{2}\{E(\lambda) + E(\lambda - 0)\} = \operatorname*{s-lim}_{\epsilon \downarrow 0} \frac{1}{2\pi i} \int_{-\infty}^{\lambda} \{R(\zeta + i\epsilon) - R(\zeta - i\epsilon)\}\, d\zeta,$$

where $E(\lambda - 0) = \text{s-lim}_{\epsilon \downarrow 0} E(\lambda - \epsilon)$. Conversely, suppose $E(\lambda)P_M = P_M E(\lambda)$ for all $\lambda \in \mathbb{R}$. For any $u \in \mathcal{H}$, one has

$$\|E(\lambda)P_M u\|_{\mathcal{H}} = \|P_m E(\lambda)u\|_{\mathcal{H}} \leq \|E(\lambda)u\|_{\mathcal{H}}$$

so, in particular, for $u \in \mathrm{Dom}\,(T)$,

$$\int_{-\infty}^{\infty} \lambda^2 \, d\|E(\lambda)P_m u\|_{\mathcal{H}}^2 \leq \int_{-\infty}^{\infty} \lambda^2 \, d\|E(\lambda)u\|_{\mathcal{H}}^2 < \infty,$$

whence $P_M u \in \mathrm{Dom}\,(T)$. Finally, for all $v \in \mathcal{H}$, we have

$$\begin{aligned} \langle v, TP_M u\rangle_{\mathcal{H}} &= \int_{-\infty}^{\infty} \lambda \, d\langle v, E(\lambda)P_M u\rangle_{\mathcal{H}} \\ &= \int_{-\infty}^{\infty} \lambda \, d\langle P_M, E(\lambda)u\rangle_{\mathcal{H}} \\ &= \langle P_M v, Tu\rangle_{\mathcal{H}} = \langle v, P_M Tu\rangle_{\mathcal{H}}, \end{aligned}$$

so $P_M T \subseteq TP_M$. □

4.2 The point spectrum and the continuous spectrum

Next we shall discuss various different decompositions of the spectrum, $\mathrm{spec}\,(T)$, for a self-adjoint operator T. The set of real numbers λ for which

$$E(\{\lambda\}) \neq 0$$

is obviously a subset of $\mathrm{spec}\,(T)$ and it called the point spectrum of T, denoted $\mathrm{spec}_{\mathrm{p}}\,(T)$. If $\lambda \in \mathrm{spec}_{\mathrm{p}}\,(T)$, then λ is an eigenvalue of T and $E(\{\lambda\})$ is the orthogonal projection onto the corresponding eigenspace. Eigenspaces corresponding to different eigenvalues μ, λ are orthogonal because $E(\{\mu\})E(\{\lambda\}) = E(\{\mu\} \cap \{\lambda\}) = 0$ and therefore $\mathrm{spec}_{\mathrm{p}}\,(T)$ is at most countable provided $\mathcal{H}$ is separable. The closure of the subspace

$$\left\{ u = \sum_{i=1}^{N} E(\{\lambda_i\})u \,:\, \lambda_i \in \mathrm{spec}\,_p(T) \right\}$$

is denoted by $\mathcal{H}_{\mathrm{p}}(T)$. Since the eigenspaces $E(\{\lambda\})\mathcal{H}$, $\lambda \in \mathrm{spec}_{\mathrm{p}}\,(T)$, reduce T, it follows from Theorem 4.1.5 that $\mathcal{H}_{\mathrm{p}}(T)$ redeuces T. Let $\mathcal{H}_{\mathrm{c}}(T) = \mathcal{H}_{\mathrm{p}}(T)^{\perp}$. Then the restrictions of T to $\mathcal{H}_{\mathrm{p}}(T)$ and $\mathcal{H}_{\mathrm{c}}(T)$ are denoted by T_{p} and T_{c}, respectively. The set $\mathrm{spec}\,(T_{\mathrm{c}})$ is called the continuous spectrum of T and it is denoted by $\mathrm{spec}_{\mathrm{c}}\,(T)$. One can express $E(\{\lambda\})$ via the unitary group and thus distinct $\mathrm{spec}_{\mathrm{p}}\,(T)$ from $\mathrm{spec}_{\mathrm{c}}\,(T)$:

Another decomposition of the spectrum of T arises by considering, for fixed $u \in \mathcal{H}$, the measure $\|E(\Omega)u\|_{\mathcal{H}}^2 = \langle u, E(\Omega)u\rangle_{\mathcal{H}} \equiv m_u(\Omega)$, where $\Omega \subseteq \mathbb{R}$ is a Borel set. In the sequel the Lebesgue measure of a Borel set Ω will be denoted by $|\Omega|$. Let $\mathcal{H}_{\mathrm{ac}}(T)$ denote the set of $u \in \mathcal{H}$ for which m_u is absolutely continuously with respect to the Lebesgue measure. That is, $u \in \mathcal{H}_{\mathrm{ac}}(T)$ if and only if $E(\Omega)u = 0$ holds for every Borel set Ω with Lebesgue measure $|\Omega| = 0$. Likewise, one can define $\mathcal{H}_{\rm s}(T)$ as the set of $u \in \mathcal{H}$ for which m_u is a singular measure with respect to the Lebesgue measure, i.e., $u \in \mathcal{H}_{\rm s}(T)$ holds if and only if there exists a Borel set Ω_0 with $|\Omega_0| = 0$ such that

$$m_u(\Omega) = m_u(\Omega \cap \Omega_0)$$

for all measurable sets Ω.

Theorem 4.2.1 *The sets $\mathcal{H}_{ac}(T)$ and $\mathcal{H}_s(T)$ are closed subspaces of $\mathcal{H}$, they are mutually orthogonal and they reduce T.*

Proof. First we show that $\mathcal{H}_{\rm ac}(T) \perp \mathcal{H}_{\rm s}(T)$. Let $u \in \mathcal{H}_{\rm ac}(T)$, $v \in \mathcal{H}_{\rm s}(T)$ and let Ω_0 be a Borel set with $|\Omega_0| = 0$ such that $m_u(\Omega) = m_v(\Omega \cap \Omega_0)$ for every measurable set Ω. Then

$$\langle u, v\rangle_{\mathcal{H}} = \langle u, E(\Omega_0)v\rangle_{\mathcal{H}} = \langle E(\Omega_0)u, v\rangle_{\mathcal{H}} = 0,$$

because $E(\Omega_0)u = 0$. Next we show that $\mathcal{H} = \mathcal{H}_{\rm ac}(T) \oplus \mathcal{H}_{\rm s}(T)$. Given $w \in \mathcal{H}$, the corresponding measure $m_w(\Omega)$ has a Lebesgue decomposition $m_w(\Omega) = m'_w(\Omega) + m''_w(\Omega)$, where m'_w is absolutely continuous with respect to the Lebesgue measure and m''_w is singular. The singular measure has support on a set Ω_0 with $|\Omega_0| = 0$. Now define the vectors $u = (1 - E(\Omega_0))w$ and $v = E(\Omega_0)w$. Then $w = u + v$ and the measure m_v is singular because

$$\begin{aligned} m_v(\Omega) &= \|E(\Omega)v\|^2_{\mathcal{H}} = \|E(\Omega)E(\Omega_0)w\|^2_{\mathcal{H}} \\ &= \|E(\Omega \cap \Omega_0)w\|^2_{\mathcal{H}} = m_w(\Omega \cap \Omega_0) \\ &= m''_w(\Omega). \end{aligned}$$

From this we see that m_u is absolutely continuous; indeed,

$$\begin{aligned} m_u(\Omega) &= \|E(\Omega)(1 - E(\Omega_0))w\|^2_{\mathcal{H}} \\ &= \|E(\Omega)w\|^2 - \|E(\Omega)E(\Omega_0)w\|^2_{\mathcal{H}} \\ &= m_w(\Omega) - m''_w(\Omega) = m'_w(\Omega). \end{aligned}$$

Thus we have shown that $u \in \mathcal{H}_{\rm ac}(T)$ and $v \in \mathcal{H}_{\rm s}(T)$. Since $\mathcal{H}_{\rm ac}(T) \perp \mathcal{H}_{\rm s}(T)$ and $\mathcal{H} = \mathcal{H}_{\rm ac}(T) \oplus \mathcal{H}_{\rm s}(T)$, the sets $\mathcal{H}_{\rm ac}(T)$ and $\mathcal{H}_{\rm s}(T)$ must be closed subspaces of $\mathcal{H}$. If $u \in \mathcal{H}_{\rm ac}(T)$, then we can show that $E(\lambda)u \in \mathcal{H}_{\rm ac}(T)$ for all $\lambda \in \mathbb{R}$ as follows. Since Ω has Lebesgue measure zero, we have

$$E(\Omega)E(\lambda)u = E(\Omega)E((-\infty, \lambda])u = E((-\infty, \lambda])E(\Omega)u = 0.$$

Denoting the orthogonal projection onto $\mathcal{H}_{\mathrm{ac}}(T)$ by $P_{\mathrm{ac}}(T)$, we infer from above that $E(\lambda)P_{\mathrm{ac}}(T) = P_{\mathrm{ac}}(T)E(\lambda)P_{\mathrm{ac}}(T)$. If $v \in \mathcal{H}_{\mathrm{s}}(T)$, then $E(\lambda)v \in \mathcal{H}_{\mathrm{s}}(T)$ because if Ω_0 is the support of m_w with $|\Omega_0| = 0$, we have that

$$E(\Omega \cap \Omega_0)E(\lambda)v = E(\Omega)E(\lambda)E(\Omega_0)v = E(\Omega)E(\lambda)v.$$

Setting $P_{\mathrm{s}} = 1 - P_{\mathrm{ac}}$, the above shows that $E(\lambda)P_{\mathrm{s}} = P_{\mathrm{s}}E(\lambda)P_{\mathrm{s}}$. In combination with the latter result, it follows that

$$E(\lambda)P_{\mathrm{ac}} = P_{\mathrm{ac}}E(\lambda)(P_{\mathrm{ac}} + P_{\mathrm{s}}) = P_{\mathrm{ac}}E(\lambda).$$

Then Theorem 4.1.5 implies that $\mathcal{H}_{\mathrm{ac}}(T)$, and thus $\mathcal{H}_{\mathrm{s}}(T)$, reduces T. $\square$

To recapitulate, any self-adjoint operator H on a Hilbert space $\mathcal{H}$ is unitarily equivalent to the operator M_f of multiplication by some real valued measurable function f on $L^2(M, d\mu)$. We define $\phi(H) = \mathcal{U}^{-1}M_{\phi\circ f}\mathcal{U}$, where $\mathcal{U} : \mathcal{H} \to L^2(M, d\mu)$ is the unitrary map that diagonalizes H.

For Borel sets $\mathfrak{B}$, let $\chi_{\mathfrak{B}}$ be the characteristic function for $\mathfrak{B}$ and denote by $E_{\mathfrak{B}}(H)$ the operator associated to $\chi_{\mathfrak{B}}$ by the functional calculus for H. For any vector $\psi \in \mathcal{H}$, the spectral theorem shows that the set function $\mu_\psi(\mathfrak{B}) = \langle \psi, E_{\mathfrak{B}}(H)\psi\rangle$ defines a positive Borel measure, called the spectral measure for ψ. Evidently,

$$\langle \psi, \phi(H)\psi\rangle = \int \phi(\lambda)\, d\mu_\psi(\lambda).$$

Theorem 4.2.2 *Let μ be a finite Bored measure on $\mathbb{R}$ and let $F(t)$ be its Fourier transform, then*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |F(t)|^2\, dt = \sum_{\lambda\in\mathbb{R}} |\mu(\lambda)|^2$$

In particular, if μ is a continuous measure the limit equals zero.

Proof. We have that $|F(t)|^2 = \displaystyle\int d\mu(\lambda)du(\lambda')e^{-it[\lambda-\lambda']}$

Since all measure one finite, then Fubini's theorem guarantees that

$$\frac{1}{T}\int_0^T |F(t)|^2 dt = \int d\mu(\lambda)d\mu(\lambda')e^{\frac{-iT(\lambda-\lambda')-1}{-iT(\lambda-\lambda')}}$$

Now, $f(x,T)$ is bounded by 1, $f(x,T) = e^{\frac{-iT(\lambda-\lambda')-1}{-iT(\lambda-\lambda')}}$.

We let $x = \lambda - \lambda'$, and then $f(x,T) = e^{\frac{-iTx-1}{-iTx}}$

if $x \neq 0$ $f(x,T)$ converges to zero as $T \to \infty$ and for $x = 0$, we have that $f(0,T) = 1$ we use l'Hopitals rule, and then by dominated convergence theorem, we have

$$\int du(\lambda)du(\lambda')f(\lambda - \lambda', T) = g(\lambda - T) \to \mu\{\lambda\}$$

as $T \to \infty$. Since $|g(\lambda, T)| \leq \mu(\mathbb{R})$, if we apply the dominated convergence theorem again, we get

$$\int d\mu(\lambda)g(\lambda,T) \to \sum_{\lambda \in \mathbb{R}} |\mu\{\lambda\}|^2$$

$\square$

Definition 4.2.3 $\mathcal{H}_{p.p}(H) = \{\psi \in \mathcal{H}, \mu_\psi$ *is a pure point measure*$\}$

$\mathcal{H}_{cont}(H) = \{\psi \in \mathcal{H}, \mu_\psi$ *is a continuos measure*$\}$.

$\mathcal{H}_{a.c}(H) = \{\{\psi \in \mathcal{H}, \mu_\psi$ *is abslutely continuos with respect to lebesgue measure*$\}$. $\mathcal{H}_{s.c.}(H) = \{\{\psi \in \mathcal{H}, \mu_\psi$ *is a singular continuous with respect to lebesque measure*$\}$

Proposition 4.2.4 *A closed bounded subset $\mathcal{S}$ of $\mathcal{H}$ is compact if and only if for every $\varepsilon > 0$, there is a finite dimensioned orthogonal projection F_ε with.*

$$\sup_{\psi \in \mathcal{S}} \|(1 - F_\varepsilon)\psi\| < \varepsilon$$

Definition 4.2.5 *We say that $\psi \in \mu_{bd}(H)$ manifold bounded state for H, if for every $\varepsilon > 0$, there is a finit dimensional orthogonal projection F_ε such that*

$\sup_t \|(1-F_\varepsilon)e^{-itH}\psi\| < \varepsilon$, $\psi \in \mu_\psi(H)$, *the manifold of states that leave any compact subset in the time if for every finite-dimensional orthogonal projection F,*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \|Fe^{-itH}\psi\|^2 dt = 0$$

Proposition 4.2.6 *For any bounded operator C, then*

1) $\lim_{T\to\infty} \frac{1}{T} \int_0^T \|Ce^{-itH}\psi\|^2 dt = 0$ *if and only if* $\lim_{T\to\infty} \frac{1}{T} \int_0^T \|Ce^{itH}\psi\| dt = 0$

2) $\frac{1}{T} \int_0^T \|Ce^{-itH}\psi\|^2 dt \leq \|C\|^2 \|\psi\|^2$

The main theorem is which such that $\mu_{bd}(H) = \mathcal{H}_{p.p}(H)$ and $\mu_{lv}(H) = \mathcal{H}_{\text{cont}}(H)$

Theorem 4.2.7 *Let H be a self-adjoint operator on the Hilbert space $\mathcal{H}$, then*

i) $\psi \in \mathcal{H}_{p.p}(H) \Leftrightarrow$ for every $\varepsilon \to 0$ there is a finite dimensional projection F_ε such that

$$\sup_{t\in\mathbb{R}} \|(1 - F_\varepsilon)e^{-itH}\psi\| < \varepsilon$$

ii) $\psi \in \mathcal{H}_{cont}(H) \Leftrightarrow$ for any finite dimensional orthogonal projection F such that

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \|Fe^{-itH}\psi\|^2 dt = 0$$

Definition 4.2.8 *A self-adjoint operator H on $L^2(R^n, d^n x)$ satisfies the local compactness property if for every pair of positive number R and E*

the operator $P_{R,E} = F(|x| \le R)F(|H| \le E)$

** $F(|x| \le R)$ is the operator of multiplication by the characteristic function of the set $\{x : |x| \le R\}$, and so*

$$F(|x| > R) = 1 - F(|x| \le R)$$

** $F(|H| \le E)$ is the spectral projection into the subspace of $\mathcal{H}$. When $|H| \le E$ the functional calculs, and so*

$$F(|H| > E) = 1 - F(|H| \le E)$$

Theorem 4.2.9 *Let H be a self-adjoint operator on $L^2(R^n, d^n x)$ with the local compactness property, then*

1) $\psi \in \mathcal{H}_{p.p}(H)$ if and only if for any $\varepsilon > 0$, there is on $\mathbb{R}$ such that

$$\sup_{t\in\mathbb{R}} \|F(|x| > R)e^{-itH}\psi\| < \varepsilon$$

2) $\psi \in \mathcal{H}_{cont}(H)$ if and only if for every positive R

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \|F(|x| \le R)e^{-itH}\psi\|^2 dt = 0$$

<u>Proof</u> ($\Longleftarrow$ suppose that $\sup_{t\in\mathbb{R}} \|F(|x| > R)e^{-itH}\psi\| < \varepsilon$) holds, let $\varepsilon > 0$, there choose R such that

$\sup_{t\in\mathbb{R}} \|(F|x| > R)e^{-itH}\psi\|\frac{1}{4}\varepsilon$ and for E such that $\|F(|H| > E)\psi\|\frac{1}{4}\varepsilon$. Now we used that $P_{R,E}$ such that $\sup_{t\in\mathbb{R}} \|1 - P_{R,E}e^{-itH}\psi\| < \frac{1}{2}\varepsilon$, and since $P_{R,E}$ is compact, so there is a finite Rank orthogonal projection called Q_ε such that $\|(1-Q_\varepsilon)P_{RE}\| < \frac{1}{2}\varepsilon$. So we defined $(1 - Q_\varepsilon) = (1 - Q_\varepsilon)P_{RE} + (1 - Q_\varepsilon)(1 - P_{RE})$, then we have that

$\sup_{t\in\mathbb{R}} \|(1 - Q_\varepsilon e^{-itH})\psi\| < \varepsilon$ therefore $\psi \in \mathcal{H}_{p.p}(H)$

$\Longleftarrow$ Let $\psi \in \mathcal{H}_{p.p}(H)$, so there is a finite Rank dimensional projection operator Q_ε for each $\varepsilon > 0$ such that $F(|x| > R) = F(|x| > R)(1 - Q_\varepsilon) + F(|x| > R)Q_\varepsilon$

Q_ε is finite Rank, we take that R large enough and so, $F(|x| > R) \to 0$ as $R \to \infty$, then $\|F(|x| > R)Q_\varepsilon\| < \dfrac{1}{2}\varepsilon$

Now apply that $F(|x| > R)$ to $e^{-itH}\psi$, then we have $\sup_{t\in\mathbb{R}} \|F(|x| > R)e^{-itH}\psi\| < \varepsilon$

$\Longleftarrow$ suppose that $\lim_{T\to\infty} \dfrac{1}{T}\displaystyle\int_0^T \|F(|x| \le R)e^{-itH}\psi\|^2 dt = 0$ hold, assume that a finit Rank projection Q Given, then, we may write Q as

$$Qe^{-itH}\psi = QF(|x| > R)e^{-itH}\psi + QF(|x| \le R)e^{-itH}\psi$$

Now, we see that the second form is bound by

$$\|QF(|x| \le R)e^{-itH}\psi\| \le \|F(|x| \le R)e^{-itH}\psi\| \longrightarrow (1)$$

and the first is $\|QF(|x| > R)e^{-itH}\psi\| \le \|QF(|x| > R)\| \longrightarrow (2)$, which we can make (1) arbitrarily small by choosing R large enough.

Now, $\lim_{T\to\infty} \dfrac{1}{T}\displaystyle\int_0^T \|F(|x| \le R)e^{-itH}\psi\|^2 dt = 0$ and by proposition 1.4.(2), we have $\|Qe^{-itH}\psi\| \to 0$ i.e. $\lim_{T\to\infty} \dfrac{1}{T}\displaystyle\int_0^T \|Qe^{-itH}\psi\| dt = 0$ and so, $\psi \in \mathcal{H}_{\text{cont}}(H)$.

$\Longleftarrow$ Let $\psi \in \mathcal{H}_{\text{cont}}(H)$, then we approximate ψ by $F(|H| \le E)\psi$, choosing E large enough, and P_{RE} by finite rank operator Q, so

$$F(|x| \le R)e^{-itH}\psi = Qe^{-itH}\psi + (P_{RE} - Q)e^{-itH}\psi + F(|x| \le R)F(|H| > E)e^{-itH}\psi$$

Here we see that the first term $\|Qe^{-itH}\psi\|$ going to zero by theorem 1.2 (2), for the two terms can be made arbitrarily smalls, so by proposition 1.4 (3) we have $\|F(|x| \le R)e^{-itH}\psi\| \to 0$.

Proposition 4.2.10 *Let $P(x,p) = f_1(x)f_2(x)$ where f_1, f_2 one positive 1 fonctions with $\displaystyle\int f_1(y)d^ny = 1$ and $\displaystyle\int f_2(y)d^ny = 1$, Let $P_t(x) = \displaystyle\int (T,P)(x,P)d^nP$ and Let $Q_t(x) = |t|^{-n}f_2(x/t)$, then $P_t(x) - Q_t(x) \to 0$ as $t \to \pm\infty$ in the sense that the difference goes to zero in $L'(R^n, d^nx)$ as $t \to \infty$*

Proof: Let the map $\mu_t : L'(\mathbb{R}^n_x) \times L'(\mathbb{R}^n_x)$

$\to L'(\mathbb{R}^n_x)$ defined by $\mu : \langle f_1, f_2\rangle \to P_1$ and satisfies $\|\mu_t\| = 1$, and Let the map $N_t : L'(\mathbb{R}^n_p)$

$\to L'(\mathbb{R}^n_x)$ defined as $N_t : f_2 \to Q_t$ satisfies $\|N_t\| = 1$

Let consider f_1, f_2 in a dense subset of $L'(\mathbb{R}^n)$ and we prove that $P_t - Q_t \to 0$ for f_1, f_2, Now let $f_1, f_2 \in \mathcal{L}(\mathbb{R}^n)$, now

$$\begin{aligned} P_t(x) &= \int d^1pf_1(x-pt)f_2(p) \\ &= |t|^{-n}\int d^1\zeta f_1(\zeta)f_2\left(\frac{x-\zeta}{t}\right) \end{aligned}$$

and since $\int d^1yf_1(y) = 1$ as above, we have

$$\begin{aligned} P_t(x) - Q_t(x) &= |t|^{-n}\int d^n\zeta f_1(\zeta)\left[f_2\left(\frac{x-z}{t}\right) - f_2(x/t)\right] \\ &= |t|^{-n}\int d^n\zeta f_1(\zeta)\int_0^1 dQ\frac{\zeta}{t}.\nabla f_2\left(\frac{x}{t} - Q\frac{\zeta}{t}\right) \end{aligned}$$

So, that

$$\begin{aligned} \|P_t - Q_t\| &\leq |t|^{-n}\int d^n\zeta\int d^nx\int_0^1 d\theta f_1(\zeta)\frac{\zeta}{t} - \nabla f_2 \\ \left(\frac{x}{t} - Q\frac{\zeta}{t}\right) &\leq |t|^{-1}\|\zeta f_1\|, \|\nabla f_2\| \end{aligned}$$

So, $\to 0$ as $t \to \pm\infty$.

Lemma 4.2.11 *The point-spectral subspace $\mathcal{H}_p(T)$ is a subspace of $\mathcal{H}_s(T)$. More precisely :*

$$\forall\mu \in \mathbb{R}, \forall u \in \mathrm{Dom}\,(T), \quad Tu = \mu u \Leftrightarrow E_T(\mu)u = u \tag{4.1}$$

Proof. We have :

$$
\begin{aligned}
\forall u \in \mathrm{Dom}\,(T), \quad \|\phi(T)u\|^2 &= \langle \phi(T)u, \phi(T)u\rangle \\
&= \int_{\lambda\in\mathbb{R}} \phi(\lambda)\, d\langle E_T(\lambda)u, \phi(T)u\rangle \\
&= \int_{\lambda\in\mathbb{R}} \phi(\lambda)\, d_\lambda \left[\int_{\mu\in\mathbb{R}} \phi(\mu)\, d_\mu\langle E_T(\lambda)u, E_T(\mu)u\rangle\right] \\
&= \int_{\lambda\in\mathbb{R}} \phi(\lambda)\, d_\lambda \left[\int_{\mu\in\mathbb{R}} \phi(\mu)\, d\langle \underbrace{E_T(\mu)E_T(\lambda)}_{=E_H(\min(\lambda,\mu))} u, u\rangle\right] \\
&= \int_{\lambda\in\mathbb{R}} \phi(\lambda)\, d_\lambda \left[\int_{\mu=-\infty}^{\lambda} \phi(\mu)\, d_\mu\langle E_T(\mu)u, u\rangle\right] \\
&= \int_{\lambda\in\mathbb{R}} \phi(\lambda)^2\, d\langle E_T(\lambda)u, u\rangle
\end{aligned}
\tag{4.2}
$$

Let u be an eigenvector of T for the eigenvalue μ. Taking $\phi(\lambda) = \lambda - \mu$ in (4.2), we obtain :

$$0 = \|(T-\mu)u\|^2 = \int_{\lambda\in\mathbb{R}} (\lambda-\mu)^2\, d\langle E_T(\lambda)u, u\rangle.$$

As $\langle E_T(\cdot), u\rangle$ is a positive measure with $\langle E_T(\mathbb{R}), u\rangle = \|u\|^2$, we have :

$$\forall \epsilon > 0, \quad E_T(]\mu-\epsilon, \mu+\epsilon[)u = u$$

that is : $E_T(\mu)u = u$. Conversely, if $E_T(\mu)u = u$, then $\langle E_T(\mathbb{R}\setminus\{\mu\})u, u\rangle = 0$ and $(T-\mu)u = 0$. $\square$

As a consequence, we have : $\mathcal{H}_{\mathrm{ac}} \subset \mathcal{H}_{\mathrm{c}}$, and we can define the *singular continuous subspace* as :

$$\mathcal{H}_{\mathrm{sc}} = \mathcal{H}_{\mathrm{c}} \ominus \mathcal{H}_{\mathrm{ac}}$$

Then we define as above $\mathcal{H}_{\mathrm{sc}}$ and $\mathrm{spec}_{\mathrm{sc}}\,(T) = \mathrm{spec}\,(T_{\mathrm{sc}})$, and we have :

$$\mathrm{spec}\,(T) = \overline{\mathrm{spec}_{\mathrm{pp}}\,(T)} \cup \mathrm{spec}_{\mathrm{ac}}(T) \cup \mathrm{spec}_{\mathrm{sc}}\,(T)$$

At this stage we have given three different decompositions of $\mathcal{H}$ expressed in terms of measure theoretical notions:

$$\mathcal{H} = \mathcal{H}_{\mathrm{p}}(T) \oplus \mathcal{H}_{\mathrm{c}}(T) = \mathcal{H}_{\mathrm{s}}(T) \oplus \mathcal{H}_{\mathrm{ac}}(T) = \mathcal{H}_{\mathrm{p}}(T) \oplus \mathcal{H}_{\mathrm{sc}}(T) \oplus \mathcal{H}_{\mathrm{ac}}(T).$$

Similarly we can express $\mathrm{spec}\,(T)$ as

$$\mathrm{spec}\,(T) = \overline{\mathrm{spec}\;_{\mathrm{p}}(T)} \cup \mathrm{spec}\;_{\mathrm{c}}(T) = \mathrm{spec}\;_{\mathrm{s}}(T) \cup \mathrm{spec}\;_{\mathrm{ac}}(T) = \overline{\mathrm{spec}\;_{\mathrm{p}}(T)} \cup \mathrm{spec}\;_{\mathrm{sc}}(T) \cup \mathrm{spec}\;_{\mathrm{ac}}(T),$$

where it is worth to note that $\mathrm{spec_p}(T)$ is not necessarily closed because, contrary to the other "spectra", it is not defined as the spectrum of an operator.

4.3 RAGE theorem

An application of the Riemann-Lebesgue lemma gives us the following result for $\mathcal{H}_{\mathrm{ac}}(T)$.

Theorem 4.3.1 *Assume that T is a self-adjoint operator on $\mathcal{H}$ and let $u \in \mathcal{H}_{ac}(T)$. Then $\exp(-itT)u$ converges weakly to zero as $|t| \to \infty$.*

Proof. Since $u \in \mathcal{H}_{\mathrm{ac}}(T)$ the spectral measure $\|E(\Omega)u\|_{\mathcal{H}}^2$, Ω being a Borel set, can be expressed by the Lebesgue integral of a non-negative, real-valued function f over the set Ω, i.e.,

$$\|E(\Omega)u\|_{\mathcal{H}}^2 = \int_\Omega f(x)\, dx,$$

(dx is the Lebesgue measure on $\mathbb{R}$). Now, an application of the Riemann-Lebesgue Lemma yields

$$\begin{aligned}\langle u, e^{-itT}u\rangle_{\mathcal{H}} &= \int_{-\infty}^{\infty} e^{-it\xi}\, d\langle u, E(\xi)u\rangle_{\mathcal{H}} \\ &= \int_{-\infty}^{\infty} e^{-it\xi} f(\xi)\, d\xi \longrightarrow 0, \qquad |t| \to \infty.\end{aligned}$$

due to $f \in L^1(\mathbb{R}, d\xi)$ because $\|f\|_{L^1} = \|u\|_{L^2}^2$. Finally, by using the polarization identity, we see that $\langle v, \exp(-itT)u\rangle_{\mathcal{H}} \to 0$ as $|t| \to \infty$. □

It is possible, however, to establish stronger results than the ones above. One of them is the RAGE theorem:

Theorem 4.3.2 (RAGE) *Let T be a self-adjoint operator and suppose $u \in \mathcal{H}_{ac}(T)$. Then:*

1.

$$\tau^{-1}\int_0^\tau \|Ke^{-itT}u\|_{\mathcal{H}}^2\, dt \longrightarrow 0 \text{ as } \tau \to \infty.$$

2. If K is relatively compact with respect to T, i.e., $K(T+i)^{-1}$ is compact, then

$$\tau^{-1}\int_0^\tau \|Ke^{-itT}u\|_{\mathcal{H}}^2\, dt \longrightarrow 0 \text{ as } \tau \to \infty.$$

3. If K is compact, then

$$\left\| \tau^{-1} \int_0^\tau e^{itT} K P_c(T) e^{-itT}\, dt \right\|_{\mathcal{B}(\mathcal{H})} \longrightarrow 0 \text{ as } \tau \to \infty.$$

For its proof, we refer to [27].

4.4 Characterization of bound states and scattering states

By means of the RAGE theorem one can give a characterization of the subspaces $\mathcal{H}_{\mathrm{p}}(T)$ and $\mathcal{H}_{\mathrm{c}}(T)$. First, however, we need a few preliminary definitions.

Let $\{F_r; r \geq 0\}$ denote a sequence of orthogonal projections, which converges strongly to the identity operator, i.e., $\text{s-lim}_{r\to\infty} F_r = I$. Define the following five subspaces of $\mathcal{H}$:

$$M_0(T) = \{\, u \in \mathcal{H} \,:\, \lim_{r\to\infty} \sup_t \|(I - F_r)e^{-itT}u\|_{\mathcal{H}} = 0 \,\}, \tag{4.3}$$

$$M_\infty^\pm(t) = \{\, u \in \mathcal{H} \,:\, \lim_{t\to\pm\infty} \|F_r e^{-itT}u\|_{\mathcal{H}} = 0, \text{ for all } r \geq 0 \,\}, \tag{4.4}$$

$$\widetilde{M}_\infty^\pm(T) = \left\{ u \in \mathcal{H} \,:\, \lim_{r\to\infty} \pm r^{-1} \int_0^{\pm r} \|F_r e^{-itT}u\|_{\mathcal{H}}\, dt = 0, \text{ for all } r \geq 0 \right\}. \tag{4.5}$$

In quantum mechanics, where T is a Schrödinger operator, the vectors in $\mathcal{H}_{\mathrm{p}}(T)$ are often called bound states and the vectors belonging to $\mathcal{H}_{\mathrm{c}}(T)$ are called scattering states; the following theorem justifies these names.

Theorem 4.4.1 *Suppose that there is a bounded operator S such that $(T+i)^{-1}S = S(T+i)^{-1}$, $\mathrm{Ran}\,(S) \subseteq \mathcal{H}$ is dense, and $F_r S P_c(T)$ is compact for all r. Then $M_0(T) = \mathcal{H}_p(T)$ and $\widetilde{M}_\infty^\pm(T) = \mathcal{H}_c(T)$. If the singular continuous spectrum, $\mathrm{spec}_{\mathrm{sc}}\,(T)$, is empty, then $M_\infty^\pm(T) = \mathcal{H}_{ac}(T)$.*

Proof. For pedagogical reasons it is convenient to divide the proof into six steps.
Step 1. Estimates, like the one in the beginning of the proof of the RAGE Theorem, show that $M_0(T)$, $M_\infty^\pm(T)$, and $\widetilde{M}_\infty^\pm(T)$ are all closed subspaces of $\mathcal{H}$.
Step 2. We show that $\mathcal{H}_{\mathrm{p}}(T) \subseteq M_0(T)$. Since $M_0(T)$ is closed, it suffices to prove this

postulate for those $u \in \mathcal{H}_{\mathrm{p}}(T)$, which are finite linear combinations of eigenvectors for T. In fact, the triangle inequality implies that it suffices to assume that u is an eigenvector, i.e., $Tu = \lambda u$. Then

$$\begin{aligned}\|(I - F_r)e^{itT}u\|_{\mathcal{H}} &= \|(I - F_r)e^{-it\lambda}u\|_{\mathcal{H}} \\ &= \|(I - F_r)u\|_{\mathcal{H}} \longrightarrow 0,\end{aligned}$$

as $r \to \infty$; independently of t, because $F_r \xrightarrow{s} I$ as $r \to \infty$.

Step 3. Herein we show that $M_0(T) \perp M_\infty^{\pm}(T)$ and $M_0(T) \perp \widetilde{M}_\infty^{\pm}(T)$. Let $u \in M_0(T)$ and $v \in M_\infty^{\pm}(T)$. Then

$$\begin{aligned}\langle u, v\rangle_{\mathcal{H}} &= \langle e^{-itT}u, e^{-itT}v\rangle_{\mathcal{H}} \\ &= \langle e^{-itT}u, F_r e^{-itT}v\rangle_{\mathcal{H}} + \langle (I - F_r)e^{-itT}u, e^{-itT}v\rangle_{\mathcal{H}} \\ &\leq \|u\|_{\mathcal{H}}\|F_r e^{-itT}v\|_{\mathcal{H}} + \|v\|_{\mathcal{H}}\|(I - F_r)e^{-itT}u\|_{\mathcal{H}}.\end{aligned}$$

By first taking r large enough and afterwards choosing t large enough, it follows that $\langle u, v\rangle_{\mathcal{H}} = 0$. Now, still letting $u \in M_0(T)$, and assuming $v \in \widetilde{M}_\infty^{\pm}(T)$ we have that

$$\begin{aligned}\langle u, v\rangle_{\mathcal{H}} &= \tau^{-1}\int_0^\tau dt\, \langle e^{-itT}u, e^{-itT}v\rangle_{\mathcal{H}} \\ &\leq \tau^{-1}\int_0^\tau dt\, \|F_r e^{-itT}v\|_{\mathcal{H}}\|u\|_{\mathcal{H}} \\ &\quad +\tau^{-1}\int_0^\tau \|(I - F_r)e^{-itT}u\|_{\mathcal{H}}\|v\|_{\mathcal{H}}.\end{aligned}$$

From this the assertion follows because we may choose r large enough and subsequently t large enough and use that the estimate $\|(I - F_r \exp(-it)u\|_{\mathcal{H}}$ is valid uniformly in t.

Step 4. We prove that $\widetilde{M}_\infty^{\pm}(T) \subseteq \mathcal{H}_{\mathrm{c}}(T)$. Hence, we need to show that

$$\lim_{\tau\to\infty} \tau^{-1}\int_0^\tau dt\, \|F_r e^{-itT}u\|_{\mathcal{H}} = 0$$

for all r when $u \in \mathcal{H}_{\mathrm{c}}(T)$. Since Ran $S \subseteq \mathcal{H}$ and S commutes with T, we have that $P_{\mathrm{c}}S = SP_{\mathrm{c}}$ and $S\mathcal{H}_{\mathrm{c}}(T)$ will be a dense subset of $\mathcal{H}_{\mathrm{c}}(T)$. Since $\widetilde{M}_\infty^{\pm}(T)$ is closed, it suffices to prove the claim on this dense subset. Let $u \in S\mathcal{H}_{\mathrm{c}}(T)$ and write $u = Sv$. Then, for any $v \in \mathcal{H}_{\mathrm{c}}(T)$, an application of the RAGE theorem yields

$$\pm\tau^{-1}\int_0^{\pm\tau} \|F_r e^{-itT}u\|_{\mathcal{H}}\, dt = \pm\tau^{-1}\int_0^{\pm\tau} \|F_r SP_{\mathrm{c}} e^{-itT}v\|_{\mathcal{H}}^2\, dt \longrightarrow 0,$$

as $\tau \to \infty$.

Step 5. The result of the previous four steps are combined: since $\mathcal{H}_{\mathrm{p}}(T) \subseteq M_0(T)$ (step 1) and $M_0(T) \perp \widetilde{M}_\infty^{\pm}(T)$ (step 2) we see that $\widetilde{M}_\infty^{\pm}(T) \subseteq \mathcal{H}_{\mathrm{c}}(T)$. Since $M_\infty^{\pm}(T) \subseteq \widetilde{M}_\infty^{\pm}(T)$ we also have $M_\infty^{\pm}(T) \subseteq \mathcal{H}_{\mathrm{c}}(T)$. By Step 4 it follows that $\widetilde{M}_\infty^{\pm}(T) \supseteq \mathcal{H}_{\mathrm{c}}(T)$. Consequently,

$$\widetilde{M}_\infty^{\pm}(T) = \mathcal{H}_{\mathrm{c}}(T)$$

and thus

$$M_0(T) = \mathcal{H}_{\mathrm{p}}(T).$$

It remains to prove the last part of the theorem.

Step 6. Suppose $\mathrm{spec}_{\mathrm{sc}}(T) = \emptyset$. Then $P_{\mathrm{ac}}(T) = P_{\mathrm{c}}$ and we need to show that $\mathcal{H}_{\mathrm{c}}(T) = M_\infty^\pm(T)$. As in Step 4 it suffices to prove the assertion for u belonging to the dense set $\mathrm{Ran}\, S \cap \mathcal{H}_{\mathrm{c}}(T)$. In that case, we may write $u = Sv$, $v \in \mathcal{H}_{\mathrm{c}}(T)$, and

$$\|F_r e^{-itT} u\|_{\mathcal{H}} = \|F_r S P_{\mathrm{c}}(T) e^{-itT} v\|_{\mathcal{H}}.$$

An earlier argument shows that, instead of considering the compact operator $F_r S P_{\mathrm{c}}$, it is enough to consider operators of rank one. Let $K = \langle f, \cdot \rangle_{\mathcal{H}} g$, where $f, g \in \mathcal{H}$, be such an operator. Then

$$\begin{aligned} \|K e^{-itT} v\|_{\mathcal{H}} &= \|\langle f, e^{-itT} v\rangle g\|_{\mathcal{H}} \\ &= |\langle f, e^{-itT} v\rangle_{\mathcal{H}}| \longrightarrow 0, \end{aligned}$$

as $t \to \infty$ due to Theorem 4.3.1. □

Notes on bibliography

We have used a number of references to write this chapter. We list them in alphabetical order: [2, 3, 4, 8, 18, 24, 27].

Chapter 5

Møller wave operators

5.1 Møller wave operators

Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. The evolution problem for the Schrödinger equation is given by

$$\begin{cases} i\frac{d}{dt}\varphi(t) = H\varphi(t) \\ \varphi(0) = \varphi_0 \end{cases} \tag{5.1}$$

If $\varphi_0 \in \mathrm{Dom}\,(H)$, the solution is given by :

$$\varphi(t) = e^{-itH}\varphi_0 = U(t)\varphi_0 \tag{5.2}$$

We usually work with the unitary group $U(t) = e^{itH}$, which satisfy :

$$\forall (s,t) \in \mathbb{R}^2, \quad e^{i(s+t)H} = e^{isH}e^{itH} \tag{5.3}$$

$$\forall \varphi \in \mathcal{H}, \forall t \in \mathbb{R}, \quad e^{itH}\varphi \text{ is defined and } \|e^{itH}\varphi\| = \|\varphi\| \tag{5.4}$$

$$\forall \varphi \in \mathcal{H}, \forall t \in \mathbb{R}, \quad \frac{d}{dt}e^{itH}\varphi = He^{itH} = e^{itH}H\varphi \tag{5.5}$$

$$\forall t \in \mathbb{R}, \quad e^{itH}H \subset He^{itH} \tag{5.6}$$

As mentioned in the introduction, we consider in scattering theory the problem (5.1) for two self-adjoint operators H_1 and H_2. Given an initial state φ_0, the solution of (5.1) for the Hamiltonian H_2 is $\varphi(t) = U_2(t)\varphi_0$, and the question scattering theory rises is the existence of states $\varphi_0^{\pm}$ such that the corresponding solutions $\varphi^{\pm}(t) = U_1(t)\varphi_0^{\pm}$ for the Hamiltonian H_1 behave like $\varphi(t)$ when $t \to \pm\infty$.

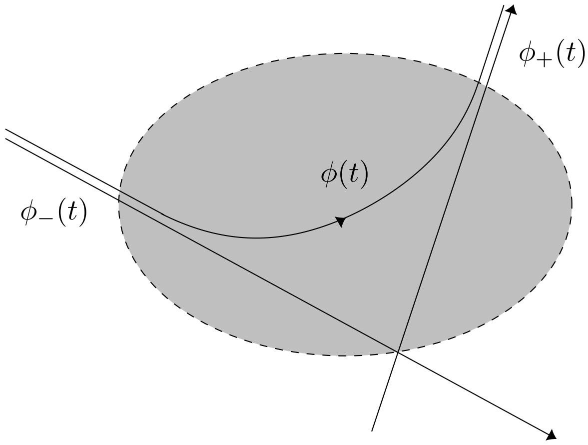

Figure 5.1: Schematic of a scattering process where the grey area indicates the support of V. Outside this interaction region, as $t \to -\infty$ the state $\psi(t)$ is approximated by $\phi_-(t)$ and likewise by $\phi_+(t)$ as $t \to \infty$.

Usually we require the norm convergence in the Hilbert space, so we actually look at the question whether

$$\|\varphi(t) - \varphi^{\pm}(t)\| = \|U_2(t)\varphi_0 - U_1(t)\varphi_0^{\pm}\| \underset{t\to\pm\infty}{\longrightarrow} 0 \tag{5.7}$$

This leads us to the operator :

$$W(t) = W(H_2, H_1; t) = U_2(-t)U_1(t) \tag{5.8}$$

and the question whether the limits

$$W_{\pm} = W_{\pm}(H_2, H_1) = \underset{t\to\pm\infty}{\text{s-lim}}\, W(H_2, H_1; t) \tag{5.9}$$

exist. But the definition we will actually use is the following :

Definition 5.1.1

$$W_{\pm} = W_{\pm}(H_2, H_1) = \lim_{t\to\pm\infty} W(H_2, H_1, t)P_1$$

where $P_j, j \in \{1, 2\}$ is the orthogonal projection onto $\mathcal{H}_{ac}(H_j)$.

Indeed, assume $\mathcal{H}_{\mathrm{p}}(H_1)$ is nonempty. Then for some $\varphi \in \mathcal{H}$ and $\lambda \in \mathbb{R}$ such that $H_1\varphi = \lambda\varphi$, we have $e^{-it(H_1-\lambda)}\varphi = \varphi$, and if W_+ exists, then for all $s \in \mathbb{R}$:

$$\|e^{is(H_2-\lambda)}\varphi - \varphi\| = \|W(t+s)\varphi - W(t)\varphi\| \underset{t\to+\infty}{\longrightarrow} 0$$

hence $e^{is(H_2-\lambda)}\varphi = \varphi$. Stone's theorem, see Theorem 3.8.2, implies $\varphi \in \mathrm{Dom}\,(H_2)$ and $H_2\varphi = \lambda\varphi$ (see [25], Section X.8). We conclude that all eigenvalues of H_1 must be eigenvalues of H_2 with the same eigenfunctions, which is wrong in general. The choice of the projection onto $\mathcal{H}_{\mathrm{ac}}(H_1)$ instead of $\mathcal{H}_s(H_1)$ is a matter of mathematical convenience and in many cases it is not important since we are interested in operators with empty singular continuous spectrum.

The following result is found in [18, Page 531, Theorem 3.2].

Proposition 5.1.2 *Suppose that wave operator $W_\pm(H, H_0, E)$ exist. Then:*

1. *$W_\pm$ is a partial isometry and is an isometry if and only if $E = 1$.*
2. *$e^{isH}W_\pm = W_\pm e^{-isH_0}$.*
3. *$\varphi(H)W_\pm = W_\pm\varphi(H_0)$.*
4. *$HW_\pm = W_\pm H_0 \qquad$ on $\mathrm{Dom}\,(H_0)$*

where
E^H is the spectral measure for H and E^{H_0} is the spectral measure for H_0.

Proof. 1). If $\psi \in E\mathcal{H}^\perp$ suth that $\psi \perp E\mathcal{H}$, Then we have, $W_\pm\psi = 0$
now, if $\psi \in \mathcal{H}$, then

$$\begin{aligned}
\|W_\pm\psi\| &= \lim_{t\to\pm\infty} \psi\|e^{itH}e^{-itH_0}E\| \\
&= \|E\psi\| \\
&= \|\psi\|
\end{aligned}$$

2).

$$\begin{aligned}
W_\pm\varphi &= s - \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\varphi \\
e^{-isH}W_\pm\varphi &= s - \lim_{t\to\pm\infty} \frac{e^{-isH}e^{itH}}{e^{i(t-s)H}}e^{-itH_0}\varphi \\
&= s - \lim_{t'\to\pm\infty} e^{it'H}e^{-it'H_0}e^{-isH_0}\varphi \\
&= s - \lim_{t'\to\pm\infty} e^{it'H}e^{-it'H_0}e^{-isH_0}\varphi \\
&= W_\pm e^{-isH_0}\varphi
\end{aligned}$$

3). For any function $\psi \in C_0^\infty(\mathbb{R})$, then the fourier transform

$$\begin{aligned}
\varphi(H)W_\pm &= \frac{1}{\sqrt{2\pi}}\int \hat{\varphi}(t)e^{iHt}dtW_\pm \\
&= \frac{1}{\sqrt{2\pi}}\int \hat{\varphi}(t)W_\pm e^{iH_0t}dt \\
&= \frac{1}{\sqrt{2\pi}}\int \hat{\varphi}(t)W_\pm e^{iH_0t}dt \\
&= W_\pm\frac{1}{\sqrt{2\pi}}\int \hat{\varphi}(t)W_\pm e^{iH_0t}dt \\
&= W_\pm\varphi(H_0)
\end{aligned}$$

Where $\varphi(H) = \dfrac{1}{\sqrt{2\pi}}\int \hat{\varphi}(t)e^{iHt}dt$

4). Consider,

$$W_\pm\frac{i}{t}(e^{-itH_0}-1)\varphi \to W_\pm H_0\varphi \qquad \text{as } t \to 0$$

For all $\varphi \in \operatorname{Dom}(H_0)$, by suing that intertwining relation as before in (iii) we have,

$$\frac{i}{t}(e^{-itH_0}-1)\varphi \to HW_\pm\varphi \qquad \text{as } t \to 0$$

and so $W_\pm\varphi \in \operatorname{Dom}(H)$ $\square$

Remark 5.1.3. The relations in items 2-4 are called the *intertwining relations* or *intertwining property*, as is the following equation

$$f(H_2)W_+ = W_+f(H_1) \tag{5.10}$$

which holds for all bounded Borel function on $\mathbb{R}$.

The following result is found in [18, Page 534, Theorem 3.5].

Proposition 5.1.4 *Let H, H_0 be self-adjoint operators on Hilbert space H, and let E be an orthogonal projection, suppose that wave operator $W_\pm(H, H_0, E)$ exists, and let $F := W_\pm W_\pm^*$ where is F final range projection. Then*

- $Fe^{-itH} = e^{-itH}F$
- *Let both $W_\pm(H_0, H, F)$ and $W_\pm(H, H_0, F)$ exist. Then*

$$W_\pm(H_0, H, F) = W_\pm(H, H_0, F)^*$$

Note that: if $E\mathcal{H} \subset \mathcal{H}_{ac}(H_0)$, then $F\mathcal{H} \subset \mathcal{H}_{ac}(H)$.

Proof. Note that: if $E\mathcal{H} \subset \mathcal{H}_{ac}(H_0)$, then $F\mathcal{H} \subset \mathcal{H}_{ac}(H)$.

- Suppose that $\varphi \in F\mathcal{H}$, it implies that $\exists\, \psi \in \mathcal{H}_{ac}(H_0)$ such that $\varphi = W_\pm(H, H_0, E)\psi$. Then,

$$\begin{aligned}
\langle \varphi, E(H)\varphi\rangle &= \langle W_\pm\psi, E(H)W_\pm\psi\rangle \\
&= \langle W_\pm\psi, W_\pm E(H_0)\psi\rangle \\
&= \langle W_\pm^* W_\pm\psi, E(H_0)\psi\rangle \\
&= \langle \psi, E(H_0)\psi\rangle
\end{aligned}$$

Since $E(H)W_\pm = W_\pm E(H_0)$ and that $W_\pm^* W_\pm = E$ is an initial range projection

- Consider that $W_\pm(H_1, H_2)W_\pm(H_2, H_1) = F_1$, then its obvious we have that $W_\pm(H_1, H_1) = F_1$, we may write that as following etc.

$W_\pm(H_2, H_1) = W_{21}$ and so $W_{12}W_{21} = F_1$, and $W_{21}W_{12} = F_2$

$$\begin{aligned}
W_{12} &= F_1 W_{12} \\
&= (W_{21}^* W_{21})W_{12} \\
&= W_{21}^*(W_{21}W_{12}) \\
&= W_{21}^*(F_2) \\
&= W_{21}^*
\end{aligned}$$

□

We now define completeness, first mentioned in the Introduction.

Definition 5.1.5 *Assume W_+ exists. Then W_+ is said to be* complete *if $N_+ = \text{Ran } W_+ = \mathcal{H}_{ac}(H_2)$. W_+ is said to be* strongly complete *if, in addition,* $\text{spec}_{\text{sc}}(H_2) = \emptyset$.

Completeness is important since the states for which we can find free asymptotics are those which lie in Ran $W_\pm$. That is why we have to know if Ran $W_\pm$ is as big as we can expect, that is if Ran $W_\pm = \mathcal{H}_{\text{ac}}(H_2)$. All the results we state concern W_+, but analogous results of course hold for W_-

The following result is found in [27, Page 19, Proposition 3].

Lemma 5.1.6 *Suppose that wave operator $W_{\pm}(H, H_0)$ exist, then they are complete if and only if $W_{\pm}(H_0, H)$ exits.*

Proof. $\Rightarrow$ Assume that $W_{\pm}(H, H_0, E_{ac}(H_0))$ are complete, then for each $\Psi \in \mathcal{H}_{a.c.}(H)$ there exists a vector $\Phi \in \mathcal{H}_{a.c.}(H_0)$ such that

$$\begin{aligned}
\Psi &= W_{\pm}(H, H_0)\Phi \\
&= \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\Phi \\
&= \lim_{t\to\pm\infty} \|e^{itH}e^{-itH_0}\Phi - \Psi\| \\
&= \lim_{t\to\pm\infty} \|e^{-itH}\Psi - e^{-itH_0}\Phi\| \\
\Phi &= s - \lim_{t\to\pm\infty} e^{itH}e^{itH_0}E_{a.c.}(H)\Psi \\
&= W_{\pm}(H_0, H)\Psi
\end{aligned}$$

$$\Phi = W_{\pm}(H_0, H, E_{ac}(H))\Psi \qquad \in \mathcal{H}_{ac}(H_0)$$

so, $W_{\pm}(H_0, H)$ exists

$\Leftarrow$ Assume that $W_{\pm}(H_0, H)$ exists , then for each $\Psi \in \mathcal{H}_{ac}(H)$ we have

$$\begin{aligned}
\Phi &= W_{\pm}(H_0, H)\Psi \\
&= \lim_{t\to\pm\infty} e^{itH_0}e^{-itH}\Psi \\
&= \lim_{t\to\pm\infty} \|e^{itH_0}e^{-itH}\Psi - \Phi\| \\
&= \lim_{t\to\pm\infty} \|e^{-itH}\Psi - e^{-itH_0}\Phi\| \\
\Psi &= s - \lim_{t\to\pm\infty} e^{itH}e^{itH_0}E_{a.c.}(H_0)\Phi
\end{aligned}$$

$$\Psi = W_{\pm}(H, H_0, E_{ac}(H_0))\Phi \qquad \in \mathcal{H}_{ac}(H)$$

so, Ran $W_{\pm}(H, H_0) = \mathcal{H}_{a.c.}(H)$ $\square$

Theorem 5.1.7 *Assume that $W_+(H_2, H_1)$ and $W_+(H_1, H_2)$ both exist. Then*

$$W_+(H_1, H_2) = W_+(H_2, H_1)^*.$$

Furthermore, $W_+(H_1, H_2)$ and $W_+(H_2, H_1)$ are both complete.

Proof. For simplicity, we write $W_{ij} = W_+(H_i, H_j)$. Using the chain rule, we get :

$$W_{12}W_{21} = W_{11} = P_1, \quad \text{and} \quad W_{21}W_{12} = P_2$$

Then, by the intertwining relations in Proposition 5.1.2, we have :

$$W_{12} = P_1 W_{12} = W_{21}^* W_{21} W_{12} = W_{21}^* P_2 = W_{21}^*$$

Then the completeness of W_{21} now follows from $W_{21}W_{12}^* = W_{21}W_{12} = P_2$ and an analogous argument works for W_{12} □

5.2 Criterion for existence of wave operators

Here we will present a general technique which is known by Cook's method. As we have stated the definitions of the wave operators and its properties above, the existence of the wave operators will be shown in most cases by cook's methods, which gives us the existence of the wave operators as defined above in Definition 3.3.

Lemma 5.2.1 *Let $(W(t))_{t\in\mathbb{R}} \subset \mathcal{B}(\mathcal{H})$ and $\varphi \in \mathcal{H}$ such that $(W(t)\varphi)_{t\in\mathbb{R}} \subset \mathcal{H}$ is strongly and such that $(t \to \|(W(t)\varphi)'\|) \in L^1(1,\infty)$*
Then, $(W(t)\varphi)_{t\in\mathbb{R}}$ is strongly convergent as $t \to +\infty$

Proof. For $\varphi \in \mathcal{H}$, then consider

$$\frac{d}{dt}W(t)\varphi = \frac{d}{dt}e^{itH}e^{-itH_0}\varphi = ie^{itH}(H - H_0)e^{-itH_0}\varphi$$

Now by integration we have

$$\begin{aligned} \|W(t)f - W(s)f\| &= \|\int_t^s \frac{d}{dt}(W(t)f)dt\| \\ &\leq \int_t^s \|(W(t)f)'dt\| \to 0 \quad \text{as } t, s \to 0 \end{aligned}$$

Since the integral is on L^1 and that $s - \lim_{t\to\infty} W(t)f$ exists, $\forall f \in \mathcal{H}$ and $W_t f$ is uniformly bounded , then $(W(t)f)_{t\in\mathbb{R}}$ is Cauchy, therefore $(W(t)f)_{t\in\mathbb{R}}$ is converge since $\mathcal{H}$ is complete in the strong topology.
$\Rightarrow (W(t)f)_{t\in\mathbb{R}}$ is convergent since $\mathcal{H}$ is complete in the strong topology.
Similar argument for t $\to -\infty$ □

Now that will lead us to we have the most important proposition about cook's methods which plays a big role in proving the existence of wave operator $W_{\pm}$. We begin with a simple criterion for existence of wave operators, going back to Cook [7] and Kuroda [19].

Theorem 5.2.2 (Cook's Criterion) *Let (H, H_0) be a pair of self-adjoint oprator on a Hilbert space $\mathcal{H}$, suppose that* $\operatorname{Dom}(H_0) = \operatorname{Dom}(H)$*, and let $V = H - H_0$. Suppose there is a dense set of vectors $\mathcal{D}$ such that $\mathcal{D} \subset \operatorname{Dom}(H_0)$.*

$$\int dt \|Ve^{-itH_0}\varphi\| < \infty \qquad \textit{for all } \varphi \in \mathcal{D}$$

Then the strong limits $W_{\pm}(H, H_0)$ exist.

Proof. Here we will show that W_+ exists, and for W_- is just similar.
first we consider that $W(t) := e^{itH}e^{itH_0}$ and then for $\varphi \in \mathcal{H}$ we have,

$$\begin{aligned}
\|W(t)\varphi - W(s)\varphi\| &= \|\int_t^s dt \frac{d}{dt} W(t)\varphi\| \\
&= \|\int_t^s dt \frac{d}{dt} e^{itH} e^{-itH_0}\varphi\| \\
&= \|\int_t^s dt e^{itH}(iH - iH_0)e^{-itH_0}\varphi\| \\
&= \|\int_t^s dt e^{itH} i(V)e^{-itH_0}\varphi\| \\
&\leq \int_t^s dt \|Ve^{-itH_0}\varphi\|
\end{aligned}$$

Since $\|e^{itH}\| = 1$, and we have used that $\operatorname{Dom}(H) = \operatorname{Dom}(H_0)$ and $e^{itH_0}\operatorname{Dom}(H_0) = \operatorname{Dom}(H_0)$ and then by the previous lemma 0.1.23 we conclude that,

$$(W(t)\varphi)_{t\in\mathbb{R}} \quad \text{is a strongly convergent}$$

$\square$

Now let apply Cook's method to the pair (H, H_0). For each Ψ there is a dense set $\mathcal{D}$ with $\|F(|\boldsymbol{x}| < a|t|)e^{-itH_0}\Psi\| \leq C(1 + |t|)^{-\mathbb{N}}$ and some $a > 0$ Then we now estimates, for $\Psi \in \mathcal{D}$

$$\begin{aligned}
&\|Ve^{-itH_0}\Psi\| \\
&\quad \leq \|V(H_0 + i)^{-1}\| \|F(|\boldsymbol{x}| < a|t|)e^{-itH_0}(H_0 + i)\Psi\| \\
&\quad + \|V(H_0 + i)^{-1}F(|\boldsymbol{x}| \geq a|t|)\| \|(H_0 + i)\Psi\|
\end{aligned}$$

The first term , first factor is obviously bounded since V is H_0-bounded and the second factor is decay in t. The second term integrable decay in t if V is decay rapidly as

$V(\boldsymbol{x}) = O(|\boldsymbol{x}|^{-(1+\epsilon)})$ as $|\boldsymbol{x}| \to \infty$ for some $\epsilon > 0$. Which this leads us to introduce the following.

The following result is found in [24, Page 38, Corollary 3.4].

Corollary 5.2.3 *Let* $\mathcal{D} = \{\Psi \in L^2(\mathbb{R}^\nu) : \hat{\Psi} \in C_0^\infty(\mathbb{R}^\nu)/\{0\}\}$. *For each* $\Psi \in \mathcal{D}$ *there is* $a > 0$ *such that*

$$\|F(|\boldsymbol{x}| < a|t|)e^{-itH_0}\Psi\| \leq C(1+|t|)^{-\mathbb{N}} \tag{5.11}$$

Definition 5.2.4 *An operator* V *is said to satisfy Enss condition if*

- V *is* H_0*-bounded with relative bound* $a < 1$.
- *The bounded, monotone decreasing function.*

$$h(R) = \|V(H_0 + i)^{-1}F(|\boldsymbol{x}| \geq R)\| \tag{5.12}$$

is integrable on $(0, \infty)$.

5.3 Closer look at incoming and outgoing states

Let $\chi_\pm$ be the characteristic function of $S_\pm$ defined by

$$S_\pm = \{\, (x(0), p(0)) \;:\; \pm x(0) \cdot p(0) > 0 \,\}$$

and let $P_\pm$ be defined by

$$(P_\pm f)(x,p) = \chi_\pm(x,p) \times f(x,p).$$

Recall the following classical fact.

Proposition 5.3.1 *Let* $\Psi \in L^2(\mathbb{R}^d, d^dx)$ *satisfy*

$$\text{supp } \widehat{\Psi} \subset \{p \in \mathbb{R}^d \;:\; |p| > a \textit{ for some } a > 0\}.$$

Let $f_\Psi(x,p)$ *be the classical state* $f_\Psi(x,p) = |\Psi(x)|^2|\Psi(p)|^2$ *and let* T *be the classical free evolution*

$$(T_t f)(x,p) = (x - pt, p).$$

Then:

(i) $(T_t P_+ f_\Psi)(x,p) = 0$ *for any* $t > 0$ *and* x *with* $|x| < a|t|$

(ii) $(T_t P_- f_\Psi)(x,p) = 0$ *for any* $t < 0$ *and* x *with* $|x| < a|t|$

Proof. We only prove (i) because (ii) can be shown in the asme way. We calculate

$$T_t P_+ f_\Psi(x,p) = \chi^t_\pm(x,p) f_\Psi(x - pt, p),$$

where $\chi^t_\pm$ is the characteristic function of the set

$$S^t_+ = \{(x,p) \,:\, (x - pt)\cdot p > 0\}$$

If $|x| < a|t|$, then $(x - pt)\cdot p \leq |p|(|x| - |p|t) < 0$ so $(T_t P_+ f_\Psi)(x,p) = 0$. □

Next we wish to prove the quantum analogue of the latter result.

Proposition 5.3.2 *Let* D *be the symmetric operator* $\frac{1}{2}(x\cdot p+p\cdot x)$ *with domain* $C^\infty_0(\mathbb{R}^d\backslash 0)$. *Then* D *has a unique self-adjoint extension with the following properties:*

1. D *has purely absolutely continuous spectrum on* $(-\infty, +\infty)$.

2. D *is diagonalized by the unitary map* $\mathcal{M} : L^2(\mathbb{R}^d, d^d x) \to L^2(\mathbb{R}) \otimes L^2(\mathbb{S}^{d-1})$ *defined by*

$$(\mathcal{M}f)(\lambda, w) = \lim_{N\to\infty} (2\pi)^{-1/2} \int_{1/N}^{N} |y|^{d/2} |y|^{-i\lambda} f(|y|, w)\, \frac{d|y|}{|y|},$$

where the limit is in the L^2 *sense. For* $f \in C^\infty_0(\mathbb{R}^d \setminus 0)$ *the formula is valid pointwise.*

3. If $\mathscr{F}$ *denotes the Fourier transform, then* $\mathscr{F} D \mathscr{F}^{-1} = -D$.

Proof. Since D is commutes with rotation, it is convenient to view $L^2(\mathbb{R}^d, dx)$ as $L^2(\mathbb{R}^+, r^{d-1}\,dr) \otimes L^2(\mathbb{S}^{d-1})$. Let $\mathcal{U}$ be the unitary map from $L^2(\mathbb{R}^+, r^{d-1}\,dr) \otimes L^2(\mathbb{S}^{d-1})$ to $L^2 \otimes L^2(\mathbb{S}^{d-1})$ given by

$$(\mathcal{U}f)(t,\omega) = e^{dt/2} f(e^t, \omega).$$

For function $f \in C^\infty_0(\mathbb{R}^d \setminus 0)$ of the form $g(r)h(\omega)$, $(\mathcal{U}f)(t,\omega)$ is in the domain of the operator $-id/dt \otimes 1$ and $\mathcal{U}Df(t,\omega) = -id/dt(\mathcal{U}f)(t,\omega)$. The set $\mathscr{S}$ of finite linear combinations of such f is dense in $L^2(\mathbb{R}^d, dx)$ and its image under $\mathcal{U}$ is a core (cf. Chapter 0) for the operator $-id/dt \otimes 1$. By unitarity, D is essentially self-adjoint on $\mathscr{S}$. Since the Fourier transform $\mathscr{F}_1$ on $L^2(\mathbb{R}, dx)$ diagonalizes the operator $-id/dt$, we set $\mathcal{M} = (\mathscr{F}_1 \otimes 1) \circ \mathcal{U}$ and obtain a map that diagonalizes D. Assertion 1 follows immediately from the unitary equivalence of D and $-id/dt \otimes 1$, and Assertion 2 follows from the corresponding facts about the Fourier transform. To prove item 3, we note that if $\mathcal{M}_j$ is the operator of multiplication by the jth coordinate and ∇_j the operator of differentiation with respect to the jth coordinate, $\mathscr{F}\mathcal{M}_j\mathscr{F}^{-1} = i\nabla_j$ and $\mathscr{F}_i\nabla_j\mathscr{F}^{-1} = \mathcal{M}_j$. Hence for any $f \in C_0^\infty(\mathbb{R}^n \setminus 0), \mathscr{F}Df = -D\mathscr{F}f$. $\square$

Theorem 5.3.3 *Let* $H_0 = -\frac{1}{2}\Delta$, *let* $D = \frac{1}{2}(x \cdot p + p \cdot x)$, *and let* $P_\pm$ *project onto the positive and negative spectral subspaces for* D. *Let real numbers* a, b *satisfy* $0 < a < b < \infty$, *and let* $g \in C_0^\infty(\mathbb{R}^+)$ *with* $\operatorname{supp} g \subset \left[\frac{a^2}{2}, \frac{b^2}{2}\right]$. *Then, for* $\pm t \in (0, \infty)$ *and* $\varepsilon > 0$, *and any positive integer* N,

$$\|F(|x| < a(1-\varepsilon)|t|)e^{-itH_0}g(H_0)P_\pm\| \leq C_{N,\varepsilon,g}(1+|t|)^{-N}. \tag{5.13}$$

Proof. Let $\Psi \in L^2$ with $\widehat{\Psi} \in C_0^\infty(\mathbb{R}^d \setminus \{0\})$ and let $\Psi_t(x) = (e^{-itH_0}g(H_0)P_\pm\Psi)(x)$. Then the pointwise formula

$$\Psi_t(x) = (2\pi)^{-d/2} \int pe^{i(p\cdot x - p^2\frac{t}{2})}g(\frac{p^2}{2})\widehat{(P_\pm\Psi)}(p)\, dp$$

holds true. We introduce $K_{x,t}(p) := (2\pi)^{-d/2}e^{-i(p\cdot x-p^2\frac{t}{2})}\overline{g(p^2/2)}$ and write

$$\Psi_t(x) = \langle K_{x,t}, \widehat{P_\pm\Psi}\rangle,$$

where $\langle\cdot,\cdot\rangle$ is the usual inner product on $L^2(\mathbb{R}^d, dp)$. An application of Proposition 5.3.2, assertion 3, yields

$$\langle K_{x,t}, \widehat{P_+\Psi}\rangle = \langle K_{x,t}, P_-\widehat{\Psi}\rangle = \langle P_-K_{x,t}, \widehat{\Psi}\rangle.$$

Next, by using Schwarz's inequality, we obtain

$$|\Psi_t(x)| \leq \|P_-K_{x,t}\|\|\widehat{\Psi}\| = \|P_-K_{x,t}\|\|\Psi\|$$

By a standard density argument, we obtain this for all $\Psi \in L^2$. If, for a moment – to be proven below – we accept the following uniform estimate, in $\pm t > 0$ and x with $|x| < a(1-\varepsilon)|t|$,

$$\|P_\mp K_{x,t}\| \leq D_{M,\varepsilon,g}(1+|t|)^{-M} \tag{5.14}$$

for any positive integer M, then we can derive (5.13) from (5.14) because the volume of the region $|x| < a(1-\varepsilon)|t|$ is bounded by a constant times $|t|^n$ (We choose $M = N + n$). $\square$

To complete the proof of Theorem 5.3.3 we prove the estimate (5.14).

Lemma 5.3.4 *One has*

$$\|P_{\mp}K_{x,t}\| \leq D_{M,\varepsilon,g}(1+|t|)^{-M}.$$

Proof. We give the proof for $t>0$ and P_- since the proof for $t<0$ and P_+ is very similar. Since $\mathcal{M}$ is unitary,

$$\|P_-K_{x,t}\| = \|\mathcal{M}P_-K_{x,t}\| = \|\chi_-(\mathcal{M}K_{x,t})\|,$$

where χ is multiplication by the characteristic function of the negative half-line in the spectral variable. The estimate (5.14) will follow from the pointwise estimate

$$|\mathcal{M}K_{x,t}(\lambda,\omega)| \leq E_{L,\epsilon,g}(1+|t|+|\lambda|)^{-L} \tag{5.15}$$

true for $\epsilon>0, t>0, |x|<a(1-\epsilon)|t|$, and any positive integer L. To prove it, we compute $(\mathcal{M}K_{x,t})(\lambda,\omega)$ and apply Hörmander's method of non-stationary phase (Theorem A.1.1 in Appendix). Compute

$$\begin{aligned}(\mathcal{M}K_{x,t})(\lambda,\omega) \quad &= \quad (2\pi)^{-(d+1)/2}\int_0^\infty |p|^{d/2}\frac{d|p|}{|p|} \\ &\quad \times|p|^{-i\lambda}e^{-(ip\cdot x-p^2t/2)}\overline{g(p^2/2)}\end{aligned}$$

and we write $|p|^{-i\lambda}e^{-(ip\cdot x-p^2t/2)} = e^{-is\phi}$ where $s=(1+|\lambda|+|t|)$ and $\phi(p,\omega)=(p\cdot x - p^2t/2+\lambda\log p)/(1+|\lambda|+|t|)$. For $\lambda<0$ and $|x|<a(1-\epsilon)|t|, |(\nabla\phi)(p,\omega)| \geq C_{\epsilon,a,b}$, so the integral has no points of stationary phase. An application of Theorem A.1.1 yields (5.15) as requested. □

We also have the following result.

Proposition 5.3.5 $P_{\mp}e^{-itH_0} \to^s 0$ *as* $t\to\pm\infty$.

Proof. Bear in mind that the vectors of the type $\Psi_{R,g}=g(H_0)F(|x|<R)\Psi$ are dense in $L^2(\mathbb{R}^d)$ as g varies over $C_0^\infty(\mathbb{R}^+)$ functions, R varies over the positive numbers, and Ψ varies over $L^2(\mathbb{R}^d)$. Taking adjoints in (5.13), we deduce that, for $\pm t\in(0,\infty)$,

$$\|P_{\mp}g(H_0)e^{-itH_0}F(|x|<a(1-\epsilon)|t|)\| \leq C_{N,\epsilon,g}(1+|t|)^{-N}.$$

Hence, for $|t|$ large enough and $\pm t\in(0,\infty)$, we obtain

$$\|P_{\mp}e^{-itH_0}\Psi_{R,g}\| = \mathcal{O}(|t|^{-N}) \text{ as } t\in\pm\infty.$$

Since the set of all such vectors is dense, we conclude that $P_{\mp}e^{-itH_0}\to^{\mathrm{s}} 0$ as $t\to\pm\infty$. □

Notes on bibliography

We have used a number of references to write this chapter. We list them in alphabetical order: [2, 3, 4, 7, 8, 18, 19, 24, 27].

Chapter 6

Classic result on asymptotic completeness

6.1 Assumptions and classic theorem

We study the scattering theory of the pair (H, H_0) where $H_0 = -\frac{1}{2}\Delta$ and the difference $H - H_0$ satisfies the Enss condition as defined below; in fact, a more general condition will be stated.

Definition 6.1.1 *The operator V is said to satisfy the Enss condition provided*

1. *The operator V is H_0-bounded with relative bound $a < 1$.*
2. *The bounded, monotone, decreasing function*

$$h(R) = \|V(H_0 + i)^{-1} F(|x| \geq R)\|$$

is integrable on $(0, \infty)$.

In this chapter we prove that the wave operators $W_\pm(H, H_0)$ are asymptotically complete by using Enss' method as described in Perry's monograph [24, Theorem 7.2].

Let F_R be "localizing operators" on a Hilbert space $\mathcal{H}$, indexed by a positive number $R \in \mathbb{R}$, i.e., (LO1) F_R is a bounded operator on $\mathcal{H}$ and $F_R^* = F_R$.

(LO2) s-$\lim_{R\to\infty} F_R = 1$.

Next we introduce the abstract local compactness property. In the sequel, for a given self-adjoint operator H, we let $G_E(H)$ denote the operator $F(|H| \le E)$ (i.e., the spectral projection onto the subspac of $\mathcal{H}$ where $|H| \le E$, defined by the functional calculus (see Section 3.6), and let $F(|H| > E) = 1 - F(|H| \le E)$).

Definition 6.1.2 *A self-adjoint operator H on a Hilbert space $\mathcal{H}$ satisfies the local compactness property if for every pair R, E of positive real numbers, the operators $P_{R,E} = F_R G_E(H)$ are compact.*

Proposition 6.1.3 *Let F_R be a family of localizing operators in the sense of (LO1)-(LO2), and let H be a self-adjoint operator on $\mathcal{H}$. Then the following are equivalent.*

1. H has the local compactness property.

2. For some fixed $g \in C_\infty(\mathbb{R})$, the continuous functions vanishing at infinity, with locally bounded inverse and all $R > 0$, $F_R g(H)$ is compact.

3. The conclusion of (b) holds for all $g \in C_\infty(\mathbb{R})$.

Proof. Suppose that assertion 1 holds. Then for $g \in C_\infty$, and for any $0 < R, E < \infty$, we have

$$\begin{aligned} F_R g(H) &= F_R P_{RE} g(H) + F(|x| \le R) F_R g(H) F(|H| > E) \\ &\quad + F(|x| > R) F_R g(H) F(|H| \le E) \\ &\quad + F(|x| > R) F_R g(H) F(|H| > E) \end{aligned}$$

The first term is compact, and the second, third, and fourth term are vanish in operator norm as $R, E \to \infty$ since $g \in C_\infty(R)$. Hence $F_R g(H)$ is compact by the norm-closed of the compact operator. This shows that assertion (1) implies (2), (3).

To see that (2) implies (1) we choose $0 < R, E < \infty$ and decompose $P_{R,E}$ into the two factors

$$P_{RE} = [F(|x| \le R) F(|H| \le E)][F_R g(H)^{-1}][g(H)^{-1} F(|H| \le E)].$$

Both first and second are compact, while the third factor is bounded since g^{-1} is locally bounded. Hence P_{RE} is compact. Since (3) implies (2), (3) implies (1). This complete the proof.

We impose the following hypotheses for the unperturbed "free" operator H_0.

Assumption 6.1.4 *Let H_0 be a self-adjoint operator in a Hilbert space $\mathcal{H}$ with domain* $\mathrm{Dom}\,(H_0)$. *Assume that*

(H1) H_0 has the (abstract) local compactness property (see Definition 6.1.2). Furthermore, $\mathrm{spec_s}\,(H_0) = \emptyset$, $\mathrm{spec_{pp}}\,(H_0)$ *has countable closure and* $\mathrm{spec_{ess}}\,(H_0) = \mathrm{spec_{ac}}(H_0) = [0, \infty)$.

(H2) There exists a closed, countable set S_{ex} containing $\mathrm{spec_{pp}}\,(H_0)$ *and such that that for every $f \in C_0^\infty(\mathrm{spec_{ac}}(H_0) \setminus S_{ex})$, there exists bounded operators $P_\pm$ satisfying*

(i) $\quad (P_+ + P_-)f(H_0) = (P_+^* + P_-^*)f(H_0) = f(H_0).$

(ii) $\quad P_\mp^* e^{-itH_0} f(H_0) \overset{s}{\to} 0$ *as* $t \to \pm\infty$.

Let H be the perturbed, self-adjoint operator in $\mathcal{H}$ with domain $\mathrm{Dom}\,(H)$. For the pair (H, H_0) we impose the following conditions.

Assumption 6.1.5 *Assume*

(H3) $(H - z)^{-1} - (H_0 - z)^{-1}$ *is compact on $\mathcal{H}$ for some z $\mathbb{C} \setminus \mathbb{R}$.*

(H4) The generalized wave operators $W_\pm(H, H_0) = \text{s-lim}_{t\to\mp\infty} e^{itH} e^{-itH_0} E_{ac}(H_0)$ *exist.*

(H5) For all $f \in C_0^\infty(\mathrm{spec_{ac}}(H_0) \setminus S_{ex})$, *the operators* $(W_\mp(H, H_0) - 1)f(H_0)P_\pm$ *are compact.*

We will establish the following, classic result on asymptotic completeness.

Theorem 6.1.6 *Let Assumption 6.1.4 and Assumption 6.1.5 hold for the pair* (H, H_0). *Then:*

1. $\mathrm{spec_{ess}}\,(H) = \mathrm{spec_{ess}}\,(H_0)$.

2. $\mathrm{spec_s}\,(H) = \emptyset$.

3. Eigenvalues of H can accumulate only in S_{ex} and eigenvalues of H not contained in S_{ex} have finite multiplicity.

4. The wave operators $W_{\pm}(H, H_0)$ exist and are complete.

It is also useful to introduce a few more hypotheses.

Assumption 6.1.7

(H6) There exists a closed, countable set S_{ex} containing $\mathrm{spec_{pp}}(H_0)$ such that for every $f \in C_0^{\infty}(\mathrm{spec_{ac}}(H_0) \setminus S_{ex})$, there exists bounded operators $P_{\pm}$ satisfying

(i) $(P_+ + P_-)f(H_0) = (P_+^* + P_-^*)f(H_0) = f(H_0)$.

(ii) *For each positive integer N, and some constant C_N and $\pm t > 0$,*

$$\|F_{a|t|}e^{-itH_0}f(H_0)P_{\pm}\| \leq C_N(1 + |t|)^{-N}.$$

(iii) $(P_+^* - P_+)f(H_0)$ *and* $(P_-^* - P_-)f(H_0)$ *are compact operators.*

(H7) For each $f \in C_0^{\infty}(\mathrm{spec_{ac}}(H_0) \setminus S)$, and for any $g \in C_0^{\infty}(\mathbb{R})$

$$\int_R^{\infty} \|g(H)(H - H_0)f(H_0)[1 - F_{R'}]\| \, dR' < \infty, \tag{6.1}$$

where $H - H_0$ is a quadratic form on $\mathrm{Dom}\,(H) \times \mathrm{Dom}\,(H_0)$.

6.2 Auxiliary results

We are going to prove the following result.

Proposition 6.2.1 *Let hypothesis (H1) of Assumption 6.1.4, hypothesis (H3) of Assumption 6.1.5 and hypotheses (H6)-(H7) of Assumption 6.1.7 hold. Then (H2), (H4) and (H5) hold.*

We will establish Proposition 6.2.1 in several, intermediate steps. Firstly, we have:

Proposition 6.2.2 *Suppose that hypothesis (H6) of Assumption 6.1.7 holds. Then (H2) is satisfied.*

Proof. It is evident that (H2)(i) holds true. The proof that (H2)(ii) is satisfied is very similar to the proof of Proposition 5.3.5 and, as a consequence, we omit it. □

To verify (H4), a set of vectors dense in $H_{\text{a.c.}}(H_0)$ are needed, together with a suitable generalization of Cook's criterion.

Hypothesis (H6) ensures the existence of suitable dense sets as we will demonstrate now.

Proposition 6.2.3 *Let hypothesis (H6) of Assumption 6.1.7 be satisfied. Assume, moreover, that*

$$\mathscr{D}_\pm \quad = \quad \{\, e^{isH_0} f(H_0) P_\pm \Phi \,:\, \Phi \in \mathcal{H},\ \pm s > 0,\ \textit{and}\ \ f \in C_0^\infty(\text{spec}_{\text{ac}}(H_0) \setminus S_{ex})\,\}.$$

Then:

i) $\mathscr{D}_\pm \subset \text{Dom}\,(H_0)$ *and* $\mathscr{D}_+$ *(resp.* $\mathscr{D}_-$*) is dense in* $\mathcal{H}_{a.c.}(H_0)$*.*

ii) For each $\Psi \in \mathscr{D}_+$ *(resp.* $\mathscr{D}_-$*) , there is a* $g \in C_0^\infty(\text{spec}_{\text{ac}}(H_0) \setminus S_{ex})$ *with* $g(H_0)\Psi = \Psi$*.*

iii) For each $\Psi \in \mathscr{D}_+$ *(resp.* $\mathscr{D}_-$*), some* $s > 0$ *(resp.* $s < 0$*) depending on* Ψ*, all* $t > s$ *(resp.* $t < s$*), some* $a > 0$ *and any positive integer* N*,*

$$\left\| F_{a|t-s|} e^{-itH_0} \Psi \right\| \leq C_N (1 + |t-s|)^{-N}.$$

Proof. In view of Proposition 6.2.2, hypothesis (H2)(ii) is satisfied. Hence, for any $f \in C_0^\infty(\text{spec}_{\text{ac}}(H_0) \setminus S_{\text{ex}})$,

$$P_\pm^*(s) f(H_0) = e^{isH_0} P_\pm^* e^{-isH_0} f(H_0) \to^s f(H_0)$$

as $s \to \pm\infty$ by (H6)(iii); the same holds true with $P_\pm$ replaced by $P_\pm^*$. This fact, the unitarity of e^{-isH_0}, and the density of $\bigcup\{\text{Ran}\ f(H_0) : f \in\in C_0^\infty(\text{spec}_{\text{ac}}(H_0) \setminus S_{\text{ex}})\}$ in $\mathcal{H}_{\text{a.c.}}$ imply that the first conclusion of the Proposition holds. Conclusion (ii) is evident from the definition of $\mathscr{D}_\pm$, and conclusion (iii) follows directly from the estimate in (H6). □

6.3 Generalized Cook's criterion

Theorem 6.3.1 *Let* H_0 *and* H *be two self-adjoint operators such that (H3) holds and let* $V = H - H_0$ *in the quadratic form sense on* $\text{Dom}\,(H) \times \text{Dom}\,(H_0)$*. Assume that there* *exist sets* $\mathscr{D}_\pm \subset \mathrm{Dom}\,(H_0)$ *with* $\mathscr{D}_\pm$ *dense in* $\mathcal{H}_{ac}(H_0)$ *such that, for each* $\Psi \in \mathscr{D}_\pm$*, any* $f \in C_0^\infty(\mathbb{R})$*, and some* s *depending on* Ψ *with* $\pm s > 0$

$$\int_s^{\pm\infty} \|f(H)Ve^{-itH_0}\Psi\|dt < \infty.$$

Then the generalized wave operators $W_\pm(H, H_0)$ *exist.*

Proof. We can use the trick of "integrating the derivative" again, just as in the original method by Cook; see Theorem 5.2.2 and its proof. We can thus conclude from the hypotheses that the vectors $f(H)e^{itH}e^{-itH_0}\psi$ have a strong limit as $t \to \pm\infty$ for each $\psi \in \mathscr{D}_\pm$. By (H3), and $f(H) - f(H_0)$ is compact for each $f \in C_0^\infty(\mathbb{R})$, so, since $e^{-itH_0} \to^w 0$ on $\mathcal{H}_{\rm ac}(H_0)$, it follows that the vectors $e^{itH}e^{-itH}f(H_0\psi)$ also have a strong limits as $t \to \pm\infty$ for each $\psi \in \mathscr{D}_\pm$ and any $f \in C_0^\infty(\mathbb{R})$. Since $\bigcup\{\mathrm{Ran}\, f(H_0) : f \in C_0^\infty(\mathbb{R})\}$ is dense in $\mathcal{H}$, the set of all vectors $f(H_0)\psi$ with $f \in C_0^\infty(\mathbb{R})$ and ψ ranging over $\mathscr{D}_+$ or $\mathscr{D}_-$ is dense in $\mathcal{H}_{\rm ac}(H_0)$. Hence, the wave operators exist. $\square$

We are now ready to establish the following result.

Proposition 6.3.2 *Let hypothesis (H1) of Assumption 6.1.4, hypothesis (H3) of Assumption 6.1.5 and hypotheses (H6)-(H7) of Assumption 6.1.7 be satisfied. Then (H4) holds, i.e., the*

Proof. We verify the hypotheses of Proposition 6.3.1 for the sets $\mathscr{D}_\pm$ introduced in Proposition 6.2.3. For $\psi \in \mathscr{D}_+$ (resp. $\psi \in \mathscr{D}_-$),

$$g(H)Ve^{-itH_0}\psi = g(H)Vf(H_0)e^{-itH_0}\Psi$$

for some $f \in\in C_0^\infty(\mathrm{spec}_{\rm ac}(H_0) \setminus S_{\rm ex})$ and we estimate as follows:

$$\begin{aligned} \left\|g(H)Vf(H_0)e^{-itH_0}\psi\right\| \;\; &\leq \;\; \left\|g(H)Vf(H_0)e^{-itH_0}\psi\right\| \left\|F_{a|t-s|}e^{-itH_0}\psi\right\| \\ &\quad + \left\|g(H)Vf(H_0)[1 - F_{a|t-s|}]\psi\right\| \|\psi\|\,. \end{aligned}$$

By virtue of Proposition 6.2.3, item (iii), the first term is integrable on the half-line $t > s$ (resp. $t < s$), and the second one is integrable on the same half-line in view of (H7). $\square$

6.4 Invariance of essential spectrum under perturbation

Next we establish the following fact.

Proposition 6.4.1 *Let hypothesis (H1) of Assumption 6.1.4 be satisfied for H_0, and let hypothesis (H3) of Assumption— 6.1.5 be satisfied for H. Then:*

1. $f(H) - f(H_0)$ is compact for all $f \in C_\infty(\mathbb{R})$.

2. $\mathrm{spec}_{\mathrm{ess}}(H) = \mathrm{spec}_{\mathrm{ess}}(H_0) = [0, \infty)$.

3. H has the local compactness property.

First, we note:

Lemma 6.4.2 *For all $z \in \mathbb{C} \setminus \mathbb{R}$, $(H - z)^{-1} - (H_0 - z)^{-1}$ is compact.*

Proof. Since the operators $A_z = (H-z)^{-1}(H+i)$ and $B_z = (H_0+i)(H_0-z)^{-1}$ are bounded for non-real z, it follows by $(H - z)^{-1} - (H_0 - z)^{-1} = A_z[(H + i)^{-1} - (H_0 + i)^{-1}]B_z$ that we need only verify compactness for $z = i$. Now,

$$(H + i)^{-1} - (H_0 + i)^{-1} = [(H + i)^{-1}V(H_0 + i)^{-1}] \times [F(|x| < n) + F|x| \geq n]$$

The first term is the product of the bounded operator $(H+i)^{-1}V$ and the compact operator $(H_0 + i)^{-1}F(|x| < n)$, while the second term is bounded in norm by $h(n)$, where $h(R)$ is the function defined in the Enss condition. Since $h(n) \to 0$ as $n \to \infty$, it follows by norm closure of the compact operators that $(H + i)^{-1}(H_0 + i)^{-1}$ is compact #. □

As a consequence of Proposition 3.4.3, we get:

Lemma 6.4.3 *The operator $f(H) - f(H_0)$ is compact for any $f \in C_\infty(\mathbb{R})$.*

Weyl's theorem [26, Theorem XIII.14], together with Lemma 6.4.2 immediately gives us conclusion 2 in Proposition 6.4.1. Instead of using Weyl's theorem, we provide a direct proof in the sequel based on two abstract results, the first one being Proposition 3.5.1.

We proceed by showing conclusion 2 of Proposition 6.4.1.

Proof of conclusion 2 in Proposition 6.4.1. By hypothesis, $\mathrm{spec}_{\mathrm{ess}}(H_0) = [0, \infty)$. Select an open interval I in $\mathbb{R} \setminus \mathrm{spec}_{\mathrm{ess}}(H_0)$ and choose $f \in C_\infty(\mathbb{R})$ with compact support in I. An application of Lemma 6.4.3, in conjunction with $f(H_0) = 0$, we infer that $f(H)$ is compact. As a consequence, $I \cap \mathrm{spec}_{\mathrm{ess}}(H) = \emptyset$. Thus $\mathrm{spec}_{\mathrm{ess}}(H) \subset \mathrm{spec}_{\mathrm{ess}}(H_0)$. On the other hand, for any open interval J in $\mathbb{R} \setminus \mathrm{spec}_{\mathrm{ess}}(H)$, and f compactly supported in J, Proposition 3.5.1 asserts that $f(H)$ is compact and, as a consequence of Lemma 6.4.3 , $f(H_0)$ is compact. Hence $J \cap \mathrm{spec}_{\mathrm{ess}}((H_0)$, so $\mathrm{spec}_{\mathrm{ess}}(H_0) \subset \mathrm{spec}_{\mathrm{ess}}(H)$. This proves the lemma. $\square$

We are now ready to establish the last claim in Proposition 6.4.1

Proof of assertion(iii) in Proposition 6.4.1. Firstly, we observe that item 1 of Proposition 6.4.1, in combination with Proposition 6.1.3, item 2, and the local compactness property of H_0, ensures that

$$F_R f(H) = F_R f(H_0) + F_R[f(H) - f(H_0)]$$

is compact. By invoking Proposition 6.1.3, item 3, H also has the local compactness property. $\square$

Before we can return to the proof of Theorem 6.1.6, we need to establish one additional auxiliary result.

Proposition 6.4.4 *Let hypothesis (H1) of Assumption 6.1.4, hypothesis (H3) of Assumption 6.1.5 and hypotheses (H6)-(H7) of Assumption 6.1.7 be satisfied. Then (H5) holds, i.e., the operators*

$$(W_\mp(H, H_0) - 1) f(H_0) P_\pm \tag{6.2}$$

are compact for each $f \in C_0^\infty(\mathrm{spec}_{\mathrm{ac}}(H_0) \setminus S_{ex})$.

Proof. The arguments applied in the proof of Proposition 6.2.3 can be re-cycled here and, therefore, we need only prove that $g(H) \times (W^* - 1) f(H_0) P_\pm$ is compact for some $g \in C_0^\infty(\mathbb{R})$ equal to 1 on supp f. For this purpose, we just need to show that the "approximates"

$$G(t) = g(H)[e^{itH} e^{-iH_0} - 1] f(H_0) P_\pm \tag{6.3}$$

are compact for each t and converge in operator norm as $t \to \pm\infty$. We write

$$\begin{aligned}[e^{itH}e^{-iH_0} - 1]f(H_0) &= e^{itH}[e^{-iH_0}f(H_0) - e^{-itH}f(H_0)] \\ &\quad +[f(H) - f(H_0)]\end{aligned}$$

and, by invoking Proposition 6.4.1, we deduce that the finite time approximants are compact. Next we verify the uniform convergence. The idea is to "integrate the derivative": first, we differentiate (6.3) and obtain the norm derivative

$$\begin{aligned}G'(t) &= e^{itH}(H)Vf(H_0)e^{-itH_0}P_\pm \\ &= e^{itH}g(H)V\tilde{f}(H_0)e^{-itH_0}f(H_0)P_\pm\end{aligned}$$

for any $\tilde{f} \in C_0^\infty(\mathrm{spec}_{\mathrm{ac}}(H_0) \setminus S_{\mathrm{ex}})$ with $\tilde{f} = 1$ on supp f . Clearly, the function $G'(t)$ is norm-continuous, and in fact norm-integrable on the half-line $\pm t > 0$:

$$\begin{aligned}\left\|G'(t)\right\| &\leq \left\|g(H)V\tilde{f}(H_0)\right\| \left\|F_{a|t|}e^{-itH_0}f(H_0)P_\pm\right\| \\ &\quad + \left\|g(H)V\tilde{f}(H_0)[1 - F_{a|t|}]\right\|.\end{aligned}$$

By hypothesis (H6), the first term is integrable. Liekwise, by hypothesis (H7) the second term is integrable. Since the approximants $G(t)$ converge in operator norm as $t \to \pm\infty$, the limiting operators are compact. □

6.5 Proof of strong asymptotic completeness

Returning to the proof of Theorem 6.1.6, we observe that the assertion 1 of Theorem 6.1.6 is merely Proposition 6.4.1, item 3. To verify conclusions 2 and 3 of Theorem 6.1.6, we just need to show that the essential spectrum of H contains only absolutely continuous spectrum and isolated eigenvalues of finite multiplicity outside of S_{ex}. Since $\mathrm{spec}_{\mathrm{ess}}(H) = \mathrm{spec}_{\mathrm{ess}}(H_0) = \mathrm{spec}_{\mathrm{ac}}(H_0)$, we have $\mathrm{spec}_{\mathrm{ess}}(H) \setminus S_{\mathrm{ex}} = \mathrm{spec}_{\mathrm{ac}}(H_0) \setminus S_{\mathrm{ex}}$.

We proceed in two steps.

Lemma 6.5.1 *$(W_\pm - 1)f(H)P_\pm$ is compact for all $f \in C_0^\infty(\mathrm{spec}_{\mathrm{ess}}(H) \setminus S_{ex})$.*

Proof. The result is an immediate consequence of the compactness of $f(H) - f(H_0)$ for $f \in C_\infty(\mathbb{R})$; a consequence of hypothesis (H3), Proposition 6.4.1, hypothesis (H5), and the fact that $\mathrm{spec}_{\mathrm{ess}}(H) \setminus S_{\mathrm{ex}}$ coincides with $\mathrm{spec}_{\mathrm{ac}}(H_0) \setminus S_{\mathrm{ex}}$. □

Next we introduce Q as the orthogonal projection onto the closed subspace of vectors orthogonal to the ranges of W_+ and W_-. Any point spectrum of infinite multiplicity or singular continuous spectrum in a bounded interval $I \subset \mathrm{spec}_{\mathrm{ess}}(H) \setminus S_{\mathrm{ex}})$ will lie in the range of the projection $E_I(H)Q$, which must therefore be infinite-dimensional. But it follows from Lemma 6.5.1 that:

Lemma 6.5.2 *The operator $E_I(H)Q$ is compact for any bounded subinterval I of* $\mathrm{spec}_{\mathrm{ess}}(H) \setminus S_{ex}$.

Proof. If we take "adjoint" in Lemma 6.5.1, we infer that $P^*_{\pm} f(H)(W^*_{\pm} - 1)$ is compact for any $f \in C_0^\infty(\mathrm{spec}_{\mathrm{ac}}(H0) \setminus S_{\mathrm{ex}})$.

Since $W^*_{\mp} Q = 0$, it follows that $P^*_{\pm} f(H)Q$ is compact for any such f. Since $(P^*_+ + P^*)f(H0) = f(H_0)$ and $f(H) - f(H_0)$ is compact, it follows that $(P^*_+ + P^*_- - 1)f(\mathcal{H})$ is compact, so $f(\mathcal{H})Q$ is compact. Hence, choosing $f = 1$ on I, it follows that $E_I(H)Q$ is compact. □

Moreover, we have :

Lemma 6.5.3 *The conclusions 2 and 3 of Theorem 6.1.6.*

Proof. Since $E_I(H)Q$ is a compact projection and, therefore, finite dimensional, its range can contain only finite point spectrum. □

It remains to prove that $\mathrm{Ran}\,(W_-) = \mathrm{Ran}\,(W_+) = \mathcal{H}_{\mathrm{ac}}(H)$.

We begin by observing that, as before, for any $\Psi \in \mathcal{H}_{\mathrm{ac}}(H)$, we have

$$e^{-itH}\Psi \to^{\mathrm{w}} 0 \text{ as } |t| \to \infty$$

by the Riemann-Lebesgue Lemma, so $Ce^{-itH}\Psi \to^{\mathrm{s}} 0$ as $|t| \to \infty$ for any compact operator C.

The latter fact is used to prove:

Lemma 6.5.4 *One has that $P_-^* e^{-itH}\psi \to^s 0$ as $t \to +\infty$ and $P_+^* e^{-itH}\psi \to^s 0$ as $t \to -\infty$ for $\psi \in \mathcal{H}_{ac}(H)$.*

Proof. We give the proof for P_-^*. Consider the dense subset $\mathcal{D}_{\mathrm{ac}}$ of $\mathcal{H}_{\mathrm{ac}}(H)$ consisting of all vectors $\psi \in \mathcal{H}_{\mathrm{ac}}(H)$ with $\psi = f(H)\psi$ for some $f \in C_0^\infty(\mathrm{spec}_{\mathrm{ess}}(H) \setminus S_{\mathrm{ex}})$. Then we have

$$\begin{aligned} P_-^* f(H) e^{-itH}\psi &= P_-^*[f(H) - f(H_0)]e^{-itH}\psi \\ &\quad + P_-^*[f(H_0)(1 - W_+^*)]e^{-it}\psi \\ &\quad + P_-^* e^{-itH_0} f(H_0) W_+^* \psi \end{aligned}$$

where, in the last step, we have used the intertwining relation for W_+^*. The first two terms go to zero by compactness and the last goes to zero by hypothesis (H2)(ii). □

Finally, we show that the wave operators are complete.

Lemma 6.5.5 *The wave operators $W_\mp$ are complete.*

Proof. We show that W_- is complete by showing that the set $\mathcal{D}_{\mathrm{ac}}$ defined above is contained in Ran W_-. Completeness follows since W_- has closed range and $\mathcal{D}_{\mathrm{ac}}$ is dense in $\mathcal{H}_{\mathrm{ac}}$. For such a ψ, let $\psi_t = e^{-itH}\psi$. We note that $\psi_t = f(H_0)\psi_t + [f(H) - f(H_0)]\psi_t$ so by Proposition 6.4.1, item 1, and (H2)(i), $[1 - (P_+ + P_-)]\psi_t \to 0$ as $t \to +\infty$. If ψ is orthogonal to Ran W_-, so are the ψ_t, but then

$$\begin{aligned} \|\psi\|^2 &= \langle \psi_t, \psi_t \rangle \\ &= \langle \psi_t, (P_+ + P_-)\psi_t \rangle + o(1) \\ &= \langle P^* \psi_t, \psi_t) + (\psi_t, (\mathbf{1} - W_-) f(H) P_+ \psi_t \rangle \\ &\quad + \langle \psi_t, W_- f(H) P_+ \psi_t \rangle + o(1) \end{aligned}$$

In the last equality, the first term goes to zero as $t \to +\infty$ by Lemma 6.5.4, the second term goes to zero as $t \to +\infty$ by the compactness of $(W_- - 1)f(H)P_+$, and the third term is identically zero since the ψ_t are orthogonal to Ran W_-. Hence $\mathcal{D}_{\mathrm{ac}} \subset$ Ran W_-. The proof for W_+ is similar. □

Part II

Asymptotic observables

Chapter 7

Results on asymptotic observables

7.1 Introduction

The Schrödinger operator describing the motion of an electron in a magnetic field is defined as follows. Let $\mathcal{A}$ be a real vector-function in $\mathbb{R}^d$ with d components. Formally, the operator corresponds to the differential expression $H(\mathcal{A})u = -(\nabla + i\mathcal{A})^2 = -\sum(\partial_j + i\mathcal{A}_j)^2$. The vector field $\mathcal{A}$ is called the magnetic potential and the matrix $\boldsymbol{B}$, $b_{jk} = \partial_j\mathcal{A}_k - \partial_k\mathcal{A}_j$ is the magnetic field itself. Definition of $H(\mathcal{A})$ as a self-adjoint operator in the Hilbert space requires certain conditions imposed on $\mathcal{A}$. If $\mathcal{A} \in L^2_{\mathrm{loc}}(\mathbb{R}^d)$, one can consider the quadratic form $\mathfrak{h}_{\mathcal{A}}[u] = \sum \|\partial_j u + i\mathcal{A}_j u\|^2_{L^2}$ first on $C_0^\infty(\mathbb{R}^d)$, an then on $H_{\mathcal{A}}$, the closure of C_0^∞ in the norm $\mathfrak{h}_{\mathcal{A}}[u]$. This form defines the operator $H(\mathcal{A})$.

Here we take a slightly different route to the magnetic Schrödinger operator. Let $H_0 = -(1/2)\Delta$ be the Laplacian on $L^2(\mathbb{R}^d;\mathbb{C})$ with domain $\mathrm{Dom}\,(H_0) = H^2(\mathbb{R}^d)$; the Sobolev space of order two.

Let $\boldsymbol{p} = -i\nabla$ be the momentum operator in $L^2(\mathbb{R}^d;\mathbb{C})$ and let $\mathcal{A} : \mathbb{R}^d \to \mathbb{R}^d$ be a vector potential $\mathcal{A}(\boldsymbol{x}) = (\mathcal{A}_1(\boldsymbol{x}), \ldots, \mathcal{A}_d(\boldsymbol{x}))$ with $\mathcal{A}_n \in L^2_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R})$. We choose the Poincaré gauge

$$\boldsymbol{x} \cdot \mathcal{A}(\boldsymbol{x}) = \mathcal{A}(\boldsymbol{x}) \cdot \boldsymbol{x} = 0 \tag{7.1}$$

and introduce

$$\operatorname{div}\, \mathcal{A}(\boldsymbol{x}) := \sum_{n=1}^{d} \partial_n \mathcal{A}_n(\boldsymbol{x}).$$

The magnetic Hamiltonian is formally given by

$$H(\mathcal{A}) = (1/2)(\boldsymbol{p} - \mathcal{A}(\boldsymbol{x}))^2 = (1/2)\left(\boldsymbol{p}^2 - 2\mathcal{A}(\boldsymbol{x}) \cdot \boldsymbol{p} + i \operatorname{div}\, \mathcal{A}(\boldsymbol{x}) + |\mathcal{A}(\boldsymbol{x})|^2\right) \tag{7.2}$$

Let $\langle \boldsymbol{x} \rangle$ be the regularized absolute value, i.e., $(1 + |\boldsymbol{x}|^2)^{\frac{1}{2}}$.

Assumption 7.1.1 *Suppose there exists $\epsilon > 0$ such that the operators*

$$\langle \boldsymbol{x} \rangle^{1+\epsilon} \mathcal{A}(\boldsymbol{x})\boldsymbol{p}, \quad \langle \boldsymbol{x} \rangle^{1+\epsilon} \operatorname{div}\, \mathcal{A}(\boldsymbol{x}), \quad \langle \boldsymbol{x} \rangle^{1+\epsilon} |\mathcal{A}(\boldsymbol{x})|^2 \tag{7.3}$$

are H_0-compact in $L^2(\mathbb{R}^d; \mathbb{C})$.

Here $\mathcal{A}(x)\boldsymbol{p}, \operatorname{div}\, \mathcal{A}(x)$, and $|\mathcal{A}(x)|^2$ are just the components of the square of the magnetic Hamiltonian i.e., we define $V_{\mathcal{A}} = -\mathcal{A}(x)\boldsymbol{p} + (i/2) \operatorname{div}\, \mathcal{A}(x) + (1/2)|\mathcal{A}(x)|^2$. However, we keep in mind the Kato-Rellich Theorem which guarantee that $H(\mathcal{A})$ is a self-adjoint operator on $\mathcal{H}$ with $\operatorname{Dom}(H(\mathcal{A})) = \operatorname{Dom}(H_0)$. Moreover,

$$\operatorname{Dom}(H_0) = \operatorname{Dom}(V_{\mathcal{A}})$$

i.e,

$$\|V_{\mathcal{A}}\| \leq a\|H_0 u\| + b\|u\| \quad u \in \operatorname{Dom}(H_0)$$

$V_{\mathcal{A}}$ is H_0- bounded with relative bounded less than 1 if and only if $V_{\mathcal{A}}(H_0 + i)$ is bdd, and $\|V_{\mathcal{A}}(H_0 + i)^{-1}\| < 1$ and so, $V_{\mathcal{A}}$ is H_0-compact if $V_{\mathcal{A}}(H_0 + i)^{-1}$ is compact.

Hence, under Assumption 7.1.1, the Kato-Rellich theorem asserts that $H(\mathcal{A})$ is a self-adjoint operator on $\mathcal{H}$ with domain $\operatorname{Dom}(H(\mathcal{A})) = \operatorname{Dom}(H_0) = H^2(\mathbb{R}^d; \mathbb{C})$. Moreover, $H(\mathcal{A})$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d; \mathbb{C})$.

7.2 Regularity

Henceforth we let $\mathcal{H} := L^2(\mathbb{R}^d, \mathbb{C})$. The generator of the dilation group associated with $H_0 = -(1/2)\Delta$ on $\mathcal{H}$ is given by

$$D = \frac{1}{2}(\boldsymbol{x} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \boldsymbol{x}) = \boldsymbol{x} \cdot \boldsymbol{p} - i\frac{d}{2} = \boldsymbol{p} \cdot \boldsymbol{x} + i\frac{d}{2}$$

and we define the operator $N = \boldsymbol{p}^2 + \boldsymbol{x}^2$ with $\mathrm{Dom}\,(N) = \mathrm{Dom}\,(H_0) \cap \mathrm{Dom}\,(\boldsymbol{x}^2)$ which allow us to make a relation link between the two operators H and D, so $\mathrm{Dom}\,(N)$ has the advantages that all relevant operators are defined on the set i.e., $e^{itH(\mathcal{A})}$ leaves $\mathrm{Dom}\,(N)$ invariance.

The following type of result on the regularity of $\exp(-iH(\mathcal{A}))$ goes back to Kato [17].

Lemma 7.2.1 *Let Assumption 7.1.1 be satisfied. Then* $\mathrm{Dom}\,(N) \subseteq \mathrm{Dom}\,(D)$ *and, moreover,*
1. $e^{-itH(\mathcal{A})}\,\mathrm{Dom}\,(N) = \mathrm{Dom}\,(N)$ *for all* $t \in \mathbb{R}$ *and, for some* $\gamma \geq 0$,

$$\|Ne^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} \leq ce^{\gamma|t|}\|N\Psi\|_{\mathcal{H}}$$

with $\Psi \in \mathrm{Dom}\,(N)$.
2. There exists a $z \in \mathbb{C}$, $\mathrm{Im}\; z \neq 0$, *such that* $(H(\mathcal{A}) - z)^{-1}\,\mathrm{Dom}\,(N) \subseteq \mathrm{Dom}\,(N)$.

Proof.
1. Let $\tilde{N} = \boldsymbol{p}^2 + \boldsymbol{x}^2 + V_{\mathcal{A}} + k$, where we introduce $V_{\mathcal{A}} = -\mathcal{A}(\boldsymbol{x})\boldsymbol{p} + (i/2)\,\mathrm{div}\;\mathcal{A}(\boldsymbol{x}) + (1/2)|\mathcal{A}(\boldsymbol{x})|^2$. For some constant $k > 0$ and we have that $\mathrm{Dom}\,(N) = \mathrm{Dom}\,(\tilde{N})$ since $\mathcal{A}(\boldsymbol{x})\boldsymbol{p}$, $\mathrm{div}\;\mathcal{A}(\boldsymbol{x})$, and $|\mathcal{A}(\boldsymbol{x})|^2$ are relatively compact perturbation of N and $N \geq 1$. $N\tilde{N}^{-1}$ and $\tilde{N}N^{-1}$ are bounded operators, there exits constants c_1 and c_2 such that

$$\|N\tilde{N}^{-1}\Psi\| \leq c_1\|\Psi\|$$

$$\|\tilde{N}N^{-1}\Psi\| \leq c_2\|\Psi\|$$

For $\Psi = \tilde{N}^{-1}\Psi' \in \mathrm{Dom}\,(N)$ or $\Psi = N^{-1}\Psi' \in \mathrm{Dom}\,(\tilde{N})$. We have

$$\|N\Psi\| \leq c_1\|\tilde{N}\Psi\|$$

$$\|\tilde{N}\Psi\| \leq c_2\|N\Psi\|$$

In other words, the norms $\|N \cdot \|$ and $\|\tilde{N} \cdot \|$, induced on $\mathrm{Dom}\,(N)$, are equivalent and, consequently, it suffices to prove the assertion for $\tilde{N}$.

We proceed by verifying the hypotheses in Theorem A.2.1 of Appendix A, i.e., we need to show that $H(\mathcal{A}) \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{-1})$ and $i[\tilde{N}, H(\mathcal{A})] \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{-1})$, where $\mathcal{H}_n$, $n = 0, \pm 1, \pm 2, \ldots$, is the scale of Hilbert spaces associated to $\tilde{N}$ (see Appendix). For $\Psi \in \mathrm{Dom}\,(N)$

$$\begin{aligned}
\langle \Psi, H(\mathcal{A})\Psi \rangle &= \langle \Psi, (\boldsymbol{p} - \mathcal{A})^2 \Psi \rangle \\
&= \langle \Psi, (\boldsymbol{p}^2 - 2\mathcal{A} \cdot \boldsymbol{p} + idiv\mathcal{A} + \mathcal{A}^2)\Psi \rangle \\
&= \langle \Psi, (\boldsymbol{p}^2 + V_{\mathcal{A}})\Psi \rangle \\
&\leq \langle \Psi, (\boldsymbol{p}^2 + V_{\mathcal{A}})\Psi \rangle + \langle \Psi, (\boldsymbol{x}^2 + k)\Psi \rangle \\
&= \langle \Psi, (\boldsymbol{p}^2 + V_{\mathcal{A}} + \boldsymbol{x}^2 + \gamma)\Psi \rangle \\
&\leq \langle \Psi, \tilde{N}\Psi \rangle
\end{aligned}$$

which shows that $H \in \mathcal{B}(H_1, H_{-1})$. Next we note that

$$\begin{aligned}
i[\tilde{N}, H] &= i[\boldsymbol{p}^2 + \boldsymbol{x}^2 + V_{\mathcal{A}} + k, (\boldsymbol{p} - \mathcal{A})^2] \\
&= i[\boldsymbol{p}^2 + \boldsymbol{x}^2 + V_{\mathcal{A}} + k, \boldsymbol{p}^2 - 2\mathcal{A} \cdot \boldsymbol{p} + i\,\mathrm{div}\ \mathcal{A} + |\mathcal{A}|^2] \\
&= i[\boldsymbol{p}^2 + \boldsymbol{x}^2 + V_{\mathcal{A}} + k, \boldsymbol{p}^2 + V_{\mathcal{A}}] \\
&= i[\boldsymbol{p}^2, \boldsymbol{p}^2] + i[\boldsymbol{p}^2, V_{\mathcal{A}}] + i[\boldsymbol{x}^2, \boldsymbol{p}^2] + i[\boldsymbol{x}^2, V_{\mathcal{A}}] \\
&\quad + i[A_{\mathcal{A}}, \boldsymbol{p}^2] + i[V_{\mathcal{A}}, V_{\mathcal{A}}] + i[k, \boldsymbol{p}^2] + i[k, V_{\mathcal{A}}] \\
&= i[\boldsymbol{x}^2, \boldsymbol{p}^2] + i[\boldsymbol{x}^2, V_{\mathcal{A}}] \\
&= i[\boldsymbol{x}^2, \boldsymbol{p}^2] + i[\boldsymbol{x}^2, -2\mathcal{A} \cdot \boldsymbol{p} + i\,\mathrm{div}\ \mathcal{A} + |\mathcal{A}|^2] \\
&= i[\boldsymbol{x}^2, \boldsymbol{p}^2] + i[\boldsymbol{x}^2, -2\mathcal{A} \cdot \boldsymbol{p}] + i[\boldsymbol{x}^2, i\,\mathrm{div}\ \mathcal{A}] + i[\boldsymbol{x}^2, |\mathcal{A}|^2]
\end{aligned}$$

Here we used that condition (7.1). Since $N + 2V_{\mathcal{A}}$ is bounded from below, there exists a constant c' such that

$$\begin{aligned}
\langle \Psi, i[\tilde{N}, H]\Psi \rangle &= \langle \Psi, 2(\boldsymbol{x} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \boldsymbol{x})\Psi \rangle \\
&\leq \langle \Psi, 2(\frac{\boldsymbol{x}^2}{2} + \frac{\boldsymbol{p}^2}{2} + \frac{\boldsymbol{p}^2}{2} + \frac{\boldsymbol{x}^2}{2})\Psi \rangle \\
&\leq \langle \Psi, 2(\boldsymbol{p}^2 + \boldsymbol{x}^2)\Psi \rangle \\
&\leq \langle \Psi, (\boldsymbol{p}^2 + \boldsymbol{x}^2)\Psi \rangle \\
&\leq \langle \Psi, (\boldsymbol{p}^2 + \boldsymbol{x}^2)\Psi \rangle + \langle \Psi, (\boldsymbol{p}^2 + \boldsymbol{x}^2 + 2V_{\mathcal{A}} + k')\Psi \rangle \\
&= \langle \Psi, (\boldsymbol{p}^2 + \boldsymbol{x}^2 + V_{\mathcal{A}})\Psi \rangle + \langle \Psi, (\boldsymbol{p}^2 + \boldsymbol{x}^2 + V_{\mathcal{A}} + k')\Psi \rangle \\
&= \langle \Psi, (\tilde{N} - k)\Psi \rangle + \langle \Psi, (\tilde{N} - k + k')\Psi \rangle \\
&\leq 2\langle \Psi, \tilde{N}\Psi \rangle + (k' - 2k)\|\Psi\|^2
\end{aligned}$$

which shows that $i[\tilde{N}, H] \in \mathcal{B}(H_1, H_{-1})$. An application of Theorem A.3.1 then yields the first claim.

2. For $\Psi \in \mathrm{Dom}\,(N)$ and $\mathrm{Im}\ z > 0$. Consider

$$(H(\mathcal{A}) - z)^{-1} = -i \int_0^\infty e^{izt} e^{-iH(\mathcal{A})t} dt.$$

Clearly, $e^{-iH(\mathcal{A})t}\,\mathrm{Dom}\,(N) = \mathrm{Dom}\,(N)$ for all t and we have $\|Ne^{-iH(\mathcal{A})t}\Psi\| \leq \|N\Psi\| e^{kt}$ for $\Psi \in \mathrm{Dom}\,(N)$ then

$$\int_0^T e^{it(z-H(\mathcal{A}))}\Psi\, dt \in \mathrm{Dom}\,(N) \qquad \text{for all} \quad T > 0.$$

then

$$\begin{aligned} \|N(H(\mathcal{A})-z)^{-1}\Psi\| &= \| -i\int_0^\infty dt e^{izt} N e^{-iH(\mathcal{A})t}\Psi\| \\ &\leq \int_0^\infty dt \|e^{izt} N e^{-iH(\mathcal{A})t}\Psi\| \\ &\leq \int_0^\infty dt e^{-(\mathrm{Im}\ z)t} e^{kt}\|N\Psi\| \\ &< \infty \end{aligned}$$

which $D \subset \mathrm{Dom}\,(N)$ for $k \geq 1$, so

$$(H(\mathcal{A})-z)^{-1}\Psi = -i\int_0^\infty e^{it(z-H(\mathcal{A}))}\, dt\Psi \in \mathrm{Dom}\,(N).$$

□

7.3 Compactness

Let $H(\mathcal{A})$, N and D be as above. Next we study compactness properties of commutators.

Lemma 7.3.1 *Let Assumption 7.1.1 hold, and let $H(\mathcal{A}), N$ and D as above. For $\Psi \in \mathrm{Dom}\,(N)$. Then the quadratic form*

$$K = i[H(\mathcal{A}), D] - 2H(\mathcal{A})$$

is defined termwise on $\mathrm{Dom}\,(N) \times \mathrm{Dom}\,(N)$*, and*

$$\begin{aligned} C &\equiv (H(\mathcal{A})-z)^{-1}K(H(\mathcal{A})-z)^{-1} \\ &= (H(\mathcal{A})-z)^{-1}(i[H(\mathcal{A}),D] - 2H(\mathcal{A}))(H(\mathcal{A})-z)^{-1} \\ &= (H(\mathcal{A})-z)^{-1}i[H(\mathcal{A}),D](H(\mathcal{A})-z)^{-1} - (H(\mathcal{A})-z)^{-1}2H(\mathcal{A})(H(\mathcal{A})-z)^{-1} \\ &= i[D,(H(\mathcal{A})-z)^{-1}] - 2H(\mathcal{A})(H(\mathcal{A})-z)^{-2} \end{aligned}$$

can be extended to a compact operator $L^2(\mathbb{R}^d;\mathbb{C})$*.*

Proof. First, we do the calculation of the following

$$\begin{aligned} i[\boldsymbol{p}^2, \boldsymbol{x}\cdot(\boldsymbol{p}-\mathcal{A})+i\frac{d}{2}] &= i[\boldsymbol{p}^2, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] \\ &= i[\boldsymbol{p}^2, \boldsymbol{x}\cdot\boldsymbol{p}] \\ &= i[\boldsymbol{p}^2, \boldsymbol{x}]\boldsymbol{p} + i\boldsymbol{x}[\boldsymbol{p}^2, \boldsymbol{p}] \\ &= 2\boldsymbol{p}^2 \end{aligned}$$

$$i[-\mathcal{A}(\boldsymbol{x})\boldsymbol{p}, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] = -d\mathcal{A}(\boldsymbol{x})\cdot\boldsymbol{p} - \text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{p}$$

$$\begin{aligned} i[\text{div } \mathcal{A}(\boldsymbol{x}), \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] &= i[i\,\text{div } \mathcal{A}(\boldsymbol{x}), \boldsymbol{x}\cdot\boldsymbol{p}] + i[i\,\text{div } \mathcal{A}(\boldsymbol{x}), i\frac{d}{2}] \\ &= -\text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{x}\boldsymbol{p} + \boldsymbol{x}\boldsymbol{p}\text{ div } \mathcal{A}(\boldsymbol{x}) - i\,\text{div } \mathcal{A}(\boldsymbol{x})\frac{d}{2} + i\frac{d}{2}\text{ div } \mathcal{A}(\boldsymbol{x}) \\ &= -\text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{x}\boldsymbol{p} + \boldsymbol{p}\boldsymbol{x}\text{ div } \mathcal{A}(\boldsymbol{x}) + i\,\text{div } \mathcal{A}(\boldsymbol{x})\frac{d}{2} + i\frac{d}{2}\text{ div } \mathcal{A}(\boldsymbol{x}) \\ &= -\text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{x}\boldsymbol{p} + \boldsymbol{p}\boldsymbol{x}\text{ div } \mathcal{A}(\boldsymbol{x}) + id\text{ div } \mathcal{A}(\boldsymbol{x}) \end{aligned}$$

$$\begin{aligned} i[|\mathcal{A}(\boldsymbol{x})|^2, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] &= i[|\mathcal{A}|^2, \boldsymbol{x}\cdot\boldsymbol{p}] + i[|\mathcal{A}|^2, i\frac{d}{2}] \\ &= i|\mathcal{A}|^2\boldsymbol{x}\boldsymbol{p} - i\boldsymbol{x}\boldsymbol{p}|\mathcal{A}|^2 + i|\mathcal{A}|^2 i\frac{d}{2} + \frac{d}{2}|\mathcal{A}|^2 \\ &= i|\mathcal{A}|^2\boldsymbol{x}\boldsymbol{p} - i(\boldsymbol{x}\boldsymbol{p}|\mathcal{A}|^2 - i|\mathcal{A}|^2\frac{d}{2}) + \frac{d}{2}|\mathcal{A}|^2 \\ &= i|\mathcal{A}|^2\boldsymbol{x}\boldsymbol{p} - i(\boldsymbol{p}\boldsymbol{x}|\mathcal{A}|^2 + i|\mathcal{A}|^2\frac{d}{2}) + \frac{d}{2}|\mathcal{A}|^2 \\ &= i|\mathcal{A}|^2\boldsymbol{x}\boldsymbol{p} - i\boldsymbol{p}\boldsymbol{x}|\mathcal{A}|^2 + d|\mathcal{A}|^2 \end{aligned}$$

Then

$$\begin{aligned} i[H(\mathcal{A}), D] - 2H(\mathcal{A}) &= i[(\boldsymbol{p}-\mathcal{A})^2, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] - 2H(\mathcal{A}) \\ &= i[\boldsymbol{p}^2 - \mathcal{A}(\boldsymbol{x})\boldsymbol{p} + (i/2)\text{ div } \mathcal{A}(\boldsymbol{x}) + (1/2)|\mathcal{A}(\boldsymbol{x})|^2, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] - 2H(\mathcal{A}) \\ &= i[\boldsymbol{p}^2, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] + i[-\mathcal{A}(\boldsymbol{x})\boldsymbol{p}, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] \\ &\quad + i[(i/2)div\mathcal{A}(\boldsymbol{x}), \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] + i[(1/2)|\mathcal{A}(\boldsymbol{x})|^2, \boldsymbol{x}\cdot\boldsymbol{p}+i\frac{d}{2}] - 2H(\mathcal{A}) \\ &= 2\boldsymbol{p}^2 - d\mathcal{A}(\boldsymbol{x})\cdot\boldsymbol{p} - \text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{p} - \text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{p} \\ &\quad - i/2 div\mathcal{A}(\boldsymbol{x})\boldsymbol{x}\boldsymbol{p} + i/2\boldsymbol{p}\boldsymbol{x}\text{ div } \mathcal{A}(\boldsymbol{x}) - 1/2d\, div\mathcal{A}(\boldsymbol{x}) \\ &\quad + i/2|\mathcal{A}|^2\boldsymbol{x}\boldsymbol{p} - i/2\boldsymbol{p}\boldsymbol{x}|\mathcal{A}|^2 + 1/2d|\mathcal{A}|^2 \\ &\quad - 2\boldsymbol{p}^2 + 2\mathcal{A}\cdot\boldsymbol{p} - i\,\text{div } \mathcal{A} - |\mathcal{A}|^2 \\ &= -d\mathcal{A}(\boldsymbol{x})\cdot\boldsymbol{p} - div\,\mathcal{A}(\boldsymbol{x})\boldsymbol{p} - \text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{p} \\ &\quad - i/2\,\text{div } \mathcal{A}(\boldsymbol{x})\boldsymbol{x}\boldsymbol{p} + i/2\boldsymbol{p}\boldsymbol{x}\text{ div } \mathcal{A}(\boldsymbol{x}) - 1/2d\text{ div } \mathcal{A}(\boldsymbol{x}) \\ &\quad + i/2|\mathcal{A}|^2\boldsymbol{x}\boldsymbol{p} - i/2\boldsymbol{p}\boldsymbol{x}|\mathcal{A}|^2 + 1/2d|\mathcal{A}|^2 \\ &\quad + 2\mathcal{A}\cdot\boldsymbol{p} - i\,\text{div } \mathcal{A} - |\mathcal{A}|^2 \end{aligned}$$

so K is defined on $\mathrm{Dom}\,(N) \times \mathrm{Dom}\,(N)$. In addition,

$$C = (H(\mathcal{A}) - z)^{-1} K (H(\mathcal{A}) - z)^{-1}$$

is clearly a compact operator, because C consists of sums and products of operators of the type $\mathcal{A} \cdot \boldsymbol{p}(H(\mathcal{A}) - z)^{-1}, \mathrm{div}\ \mathcal{A}(\boldsymbol{x})\boldsymbol{x} \cdot \boldsymbol{p}(H(\mathcal{A}) - z)^{-1}, |\mathcal{A}(\boldsymbol{x})|^2 (H(\mathcal{A}) - z)^{-1}$, and so which in view of Assumption 7.1.1, are all compact in $L^2(\mathbb{R}^d, \mathbb{C})$ □

7.4 Auxiliary results

Recall $\mathcal{H} = L^2(\mathbb{R}^d; \mathbb{C})$.

Lemma 7.4.1 *Let Assumption 7.1.1 hold. If* $\Psi \in \mathrm{Dom}\,(H(\mathcal{A}))$*, then there exists a real family of vectors* $\{\Psi_\alpha : \alpha > 0\} \subseteq \mathrm{Dom}\,(N) \cap \mathrm{Dom}\,(H(\mathcal{A}))$ *such that*
(P1) $\|\Psi - \Psi_\alpha\|_{\mathcal{H}} \to 0$ *as* $\alpha \to \infty$
(P2) $\|H(\mathcal{A})(\Psi - \Psi_\alpha)\|_{\mathcal{H}} \to 0$ *as* $\alpha \to \infty$

Proof. We need to prove the assertion for H_0 because the graph norms $\|H(\mathcal{A}) \cdot \|$ and $\|H_0 \cdot \|$ are equivalent. For given $\Psi \in \mathrm{Dom}\,(H_0)$, we set

$$\Psi_\alpha(\boldsymbol{x}) = (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \Psi(\boldsymbol{x}), \quad for \quad \alpha > 0$$

Then Ψ_α clearly belongs to $\mathrm{Dom}\,(\boldsymbol{x}^2)$ and, furthermore, $\Psi_\alpha \in \mathrm{Dom}\,(H_0)$. Then if $\Psi \in \mathscr{S}(\mathbb{R}^d, \mathbb{C})$. Since $\mathscr{S}(\mathbb{R}^d, \mathbb{C})$ is an operator core for $H(\mathcal{A})$, one can find a sequence of function $\Psi_m \in \mathscr{S}(\mathbb{R}^d, \mathbb{C})$ which converges to Ψ in the graph norm $\| \cdot \|^2_{H(\mathcal{A})} = \|H(\mathcal{A}) \cdot \|^2 + \| \cdot \|^2$. We verify that

$$\begin{aligned}
\boldsymbol{p}^2 (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \Phi(\boldsymbol{x}) &= -\Delta (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \Phi(\boldsymbol{x}) \\
&= -\nabla \cdot \nabla (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \Phi(\boldsymbol{x}) \\
&= -\nabla [\nabla (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \Phi(\boldsymbol{x}) + (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \nabla \Phi(\boldsymbol{x})] \\
&= -\Delta (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \Phi(\boldsymbol{x}) - \nabla (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \nabla \Phi(\boldsymbol{x}) \\
&\quad -\nabla (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \nabla \Phi(\boldsymbol{x}) - (1 + |\boldsymbol{x}|^2/\alpha)^{-1} \Delta \Phi(\boldsymbol{x}) \\
&= -\Phi(\boldsymbol{x}) \Delta [(1 + |\boldsymbol{x}|^2/\alpha)^{-1}] - 2\nabla [(1 + |\boldsymbol{x}|^2/\alpha)^{-1}] \cdot (\nabla \Phi)(\boldsymbol{x}) \\
&\quad -(1 + |\boldsymbol{x}|^2/\alpha)^{-1} (\Delta \Phi)(\boldsymbol{x})
\end{aligned}$$

$$\begin{aligned}
&-2\mathcal{A}\cdot\boldsymbol{p}(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi \\
&\quad = \quad i2\mathcal{A}(\boldsymbol{x})\nabla(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi(\boldsymbol{x}) + i2\mathcal{A}(\boldsymbol{x})(1+|\boldsymbol{x}|^2/\alpha)^{-1}\nabla\Phi(\boldsymbol{x})
\end{aligned}$$

and then we have

$$\begin{aligned}
&H(\mathcal{A})(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi = (\boldsymbol{p}-\mathcal{A})^2(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi \\
&= \quad (\boldsymbol{p}^2 - 2\mathcal{A}\cdot\boldsymbol{p} + i\,\mathrm{div}\;\mathcal{A} + |\mathcal{A}|^2)(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi \\
&= \quad \boldsymbol{p}^2(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi - 2\mathcal{A}\cdot\boldsymbol{p}(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi \\
&+ \quad i\,\mathrm{div}\;\mathcal{A}(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi + |\mathcal{A}|^2(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi \\
&= \quad -\Phi(\boldsymbol{x})\Delta[(1+|\boldsymbol{x}|^2/\alpha)^{-1}] - 2\nabla[(1+|\boldsymbol{x}|^2/\alpha)^{-1}]\cdot(\nabla\Phi)(\boldsymbol{x}) \\
&\qquad -(1+|\boldsymbol{x}|^2/\alpha)^{-1}(\Delta\Phi)(\boldsymbol{x}) \\
&+ \quad i2\mathcal{A}(\boldsymbol{x})\nabla(1+|\boldsymbol{x}|^2/\alpha)^{-1}\alpha\Phi(\boldsymbol{x}) + i2\mathcal{A}(\boldsymbol{x})(1+|\boldsymbol{x}|^2/\alpha)^{-1}\nabla\Phi(\boldsymbol{x}) \\
&+ \quad i\,\mathrm{div}\;\mathcal{A}(\boldsymbol{x})(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi(\boldsymbol{x}) + |\mathcal{A}|^2(\boldsymbol{x})(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Phi(\boldsymbol{x}) \qquad (*)
\end{aligned}$$

where all functions $(1+|\boldsymbol{x}|^2/\alpha)^{-1}, \nabla[(1+|\boldsymbol{x}|^2/\alpha)^{-1}], \Delta[(1+|\boldsymbol{x}|^2/\alpha)^{-1}], \mathrm{div}\;\mathcal{A}(\boldsymbol{x})(1+|\boldsymbol{x}|^2/\alpha)^{-1}$, and $\mathcal{A}(\boldsymbol{x})\nabla(1+|\boldsymbol{x}|^2/\alpha)^{-1}$ etc act as bounded operators. If one sets $\Phi = \Psi_n - \Psi_m$ and uses that $\{\Psi_m\} \subseteq \mathscr{S}(\mathbb{R}^d, \mathbb{C})$ is a Cauchy sequence in the graph norm, then

$$\begin{array}{cc}
\|\Psi_n - \Psi_m\|_{\mathcal{H}} \longrightarrow 0 & \|\,\mathrm{div}\;\mathcal{A}(\Psi_n - \Psi_m)\|_{\mathcal{H}} \longrightarrow 0 \\
\|\nabla(\Psi_n - \Psi_m)\|_{\mathcal{H}} \longrightarrow 0 & \|\mathcal{A}(\Psi_n - \Psi_m)\|_{\mathcal{H}} \longrightarrow 0 \\
\|\Delta(\Psi_n - \Psi_m)\|_{\mathcal{H}} \longrightarrow 0 & \||\mathcal{A}|^2(\Psi_n - \Psi_m)\|_{\mathcal{H}} \longrightarrow 0
\end{array}$$

for $n, m \to \infty$. This shows that the sequence $\{\Psi_{\alpha,m}\}$ is a Cauchy sequence in the graph norm. So $(*)$ is valid for all $\Phi \in \mathrm{Dom}\,(H_0)$. Now it remains to show that the properties (P1) and (P2) hold. For fixed $\boldsymbol{x} \in \mathbb{R}^d$,

$$(1+|\boldsymbol{x}|^2/\alpha)^{-1}\Psi(\boldsymbol{x}) \to \Psi(\boldsymbol{x}), \quad \alpha \to \infty$$

Furthermore,

$$\begin{aligned}
|\Psi(\boldsymbol{x}) - \Psi_\alpha(\boldsymbol{x})|^2 &= |\Psi(\boldsymbol{x}) - (1+|\boldsymbol{x}|^2/\alpha)^{-1}\Psi(\boldsymbol{x})|^2 \\
&= |(1-(1+|\boldsymbol{x}|^2/\alpha)^{-1})\Psi(\boldsymbol{x})|^2 \\
&= |1-(1+|\boldsymbol{x}|^2/\alpha)^{-1}|^2|\Psi(\boldsymbol{x})|^2 \\
&\leq |\Psi(\boldsymbol{x})|^2
\end{aligned}$$

which is integrable. It follows from Lebesgue's theorem on dominated convergence that $\|\Psi - \Psi_\alpha\|_{L^2} \to 0$ as $\alpha \to \infty$. Next, $\|H_0(\Psi - \Psi_\alpha)\|_{\mathcal{H}} \to 0$ follows from $(*)$ since $(1+$

$|\boldsymbol{x}|^2/\alpha)^{-1}$, as shown above, converges strongly to the identity, while $\nabla(1+|\boldsymbol{x}|^2/\alpha)^{-1}$, $\Delta(1+|\boldsymbol{x}|^2/\alpha)^{-1}$ and div $\mathcal{A}(1+|\boldsymbol{x}|^2/\alpha)^{-1}$ etc are bounded operators, which converge strongly to zero. □

Lemma 7.4.2 *Let Assumption 7.1.1 hold. Then* $\mathrm{Dom}\,(H(\mathcal{A})^2)$ *is dense in* $\mathcal{H}_c(H(\mathcal{A}))$.

Proof. Let $H(\mathcal{A})_\mathrm{c}$ be the restriction of $H(\mathcal{A})$ to $\mathcal{H}_\mathrm{c}(H(\mathcal{A}))$. Then $\mathrm{spec}\,(H(\mathcal{A})_\mathrm{c}) = \mathrm{spec}_\mathrm{c}\,(H(\mathcal{A})) \subseteq [0,\infty)$. Since $\mathrm{Dom}\,(H(\mathcal{A})_\mathrm{c}) \subseteq \mathcal{H}_\mathrm{c}(H(\mathcal{A}))$ is dense, we need to show that $(H(\mathcal{A})_\mathrm{c}+1)^{-1}\,\mathrm{Dom}\,(H(\mathcal{A})_\mathrm{c})$ is dense. Then

$$
\begin{aligned}
0 &= \langle \Phi, (H(\mathcal{A})_\mathrm{c}+1)^{-1}\Psi\rangle_{\mathcal{H}} \\
&= \langle (H(\mathcal{A})_\mathrm{c}^*+1)^{-1}\Phi, \Psi\rangle_{\mathcal{H}} \\
&= \langle (H(\mathcal{A})_\mathrm{c}+1)^{-1}\Phi, \Psi\rangle_{\mathcal{H}}
\end{aligned}
$$

for all $\Psi \in \mathrm{Dom}\,(H(\mathcal{A})_\mathrm{c})$. Therefore, $(H(\mathcal{A})_\mathrm{c}+1)^{-1}\Phi = 0$ and thus $\Phi = 0$. □

Theorem 7.4.3 *Let Assumption 7.1.1 hold. Let* $g \in C_0^\infty(\mathbb{R})$ *and* $\Psi \in \mathcal{H}_c(H(\mathcal{A}))$. *Then*

$$
\lim_{t\to\infty} \|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} = 0. \tag{7.4}
$$

Proof. First we estimate as follows,

$$
\begin{aligned}
&\|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} \\
&= \|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} \\
&- \|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}\Psi'\|_{\mathcal{H}} + \|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}\Psi'\|_{\mathcal{H}} \\
&\le \|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}(\Psi-\Psi')\|_{\mathcal{H}} + \|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}\Psi'\|_{\mathcal{H}} \\
&\le 2\|g\|_{L^\infty}\|\Psi-\Psi'\|_{\mathcal{H}} + \|\{g(D/t) - g(2H(\mathcal{A}))\}e^{-itH(\mathcal{A})}\Psi'\|_{\mathcal{H}}
\end{aligned}
$$

Now it is enough to shows that claim for Ψ belonging to a dense subset of $\mathcal{H}_\mathrm{c}(H(\mathcal{A}))$. The set $\mathrm{Dom}' = (H(\mathcal{A})-z)^{-1}\,\mathrm{Dom}\,(N)$ is dense in $\mathcal{H}$. Since $\mathrm{Dom}\,(N^2)$ is dense in $\mathcal{H}$ and $(H(\mathcal{A})-z)\,\mathrm{Dom}\,(N^2) \subseteq \mathrm{Dom}\,(N)$. For $\Psi \in \mathrm{Dom}\,(H(\mathcal{A})^2) \cap \mathcal{H}_\mathrm{c}(H(\mathcal{A}))$ one can thus find $\Psi' = (H(\mathcal{A})-z)^{-1}\Phi$, where $\Phi \in \mathrm{Dom}\,(N)$ so that

$$
\|\Psi - \Psi'\|_{\mathcal{H}} < \epsilon. \tag{7.5}
$$

We require good approximation by

$$\|(H(\mathcal{A})-z)2P_p(H(\mathcal{A}))\Psi'\|_{\mathcal{H}} < \epsilon, \tag{7.6}$$

where $P_p(H(\mathcal{A}))$ is the orthogonal projection onto the bound states. To construct Ψ' one applies Lemma 7.4.1, since $\Psi \in \mathrm{Dom}\,(H(\mathcal{A})^2)$ one has $\Phi \equiv (H(\mathcal{A})-z)\Psi \in \mathrm{Dom}\,(H(\mathcal{A}))$. Therefore on can find a sequence $\{\Phi_\alpha : \alpha > 0\}$ so that $\Phi_\alpha \in \mathrm{Dom}\,(N)$ for all $\alpha > 0$ and

$$\|\Phi - \Phi_\alpha\|_{\mathcal{H}} \longrightarrow 0, \quad \|H(\mathcal{A})(\Phi - \Phi_\alpha)\|_{\mathcal{H}} \longrightarrow 0, \quad \alpha \longrightarrow \infty$$

by choosing $\alpha_0 > 0$ such that

$$\|\Phi - \Phi_\alpha\|_{\mathcal{H}} < \epsilon / \|(H(\mathcal{A})-z)^{-1}\|_{\mathcal{B}(\mathcal{H})}, \quad \alpha > \alpha_0,$$

then

$$\begin{aligned}
\|\Psi - (H(\mathcal{A})-z)^{-1}\Phi_\alpha\|_{\mathcal{H}} &= \|(H(\mathcal{A})-z)^{-1}\Phi - (H(\mathcal{A})-z)^{-1}\Phi_\alpha\|_{\mathcal{H}} \\
&= \|(H(\mathcal{A})-z)^{-1}(\Phi - \Phi_\alpha)\|_{\mathcal{H}} \\
&\leq \|(H(\mathcal{A})-z)^{-1}\|_{\mathcal{B}(\mathcal{H})}\|\Phi - \Phi_\alpha\|_{\mathcal{H}} \\
&= \|(H(\mathcal{A})-z)^{-1}\|_{\mathcal{B}(\mathcal{H})}\frac{\epsilon}{\|(H(\mathcal{A})-z)^{-1}\|_{\mathcal{B}(\mathcal{H})}} \\
&< \epsilon
\end{aligned}$$

Furthermore, one sees that

$$\begin{aligned}
\|(H(\mathcal{A})-z)^2(\Psi - (H(\mathcal{A})-z)^{-1})\Phi_\alpha\|_{\mathcal{H}} &= \|(H(\mathcal{A})-z)^2\Psi - (H(\mathcal{A})-z)\Phi_\alpha\|_{\mathcal{H}} \\
&= \|(H(\mathcal{A})-z)^2(H(\mathcal{A})-z)^{-1}\Phi - (H(\mathcal{A})-z)\Phi_\alpha\|_{\mathcal{H}} \\
&= \|(H(\mathcal{A})-z)\Phi - (H(\mathcal{A})-z)\Phi_\alpha\|_{\mathcal{H}} \\
&= \|(H(\mathcal{A})-z)(\Phi - \Phi_\alpha)\|_{\mathcal{H}} \\
&< \epsilon \qquad\qquad \alpha > \alpha_0
\end{aligned}$$

provided α_0 is chosen large enough. Since

$$\|(H(\mathcal{A})-z)(\Phi-\Phi_\alpha)\|_{\mathcal{H}}^2 = \|(H(\mathcal{A})-z)P_p(H(\mathcal{A}))(\Phi-\Phi_\alpha)\|_{\mathcal{H}}^2 + \|(H(\mathcal{A})-z)P_c(H(\mathcal{A}))(\Phi-\Phi_\alpha)\|_{\mathcal{H}}^2,$$

one infers that $(H(\mathcal{A})-z)^{-1}\Phi_\alpha$ satisfy both 7.5 and 7.6 when $\alpha > \alpha_0$.

The first estimate shows that is bounded by $2\|g\|_{L^\infty}$ if one replace Ψ by $\Psi_\alpha \equiv (H-z)^{-1}\Phi_\alpha$ in first item. For the second term its expresses the operators $g(D/t)$ and $g(2H(\mathcal{A}))$ by the Fourier integrals

$$g(D/t) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} \hat{g}(\sigma) e^{i\sigma D/t} d\sigma \tag{7.7}$$

and

$$g(2H(\mathcal{A})) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} \hat{g}(\sigma) e^{i\sigma 2H(\mathcal{A})} d\sigma \tag{7.8}$$

and so

$$g(D/t) - g(2H(\mathcal{A})) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} d\sigma \hat{g}(\sigma) \{e^{i\sigma D/t} - e^{i\sigma 2H(\mathcal{A})}\}$$

and apply

$$e^{i\sigma A} - e^{i\sigma B} = i\sigma \int_0^1 e^{i\sigma(1-s)A}(A-B)e^{i\sigma s B} ds, \tag{7.9}$$

Now we estimate.

$$\begin{aligned}
&\|\{g(D/t) - g(2H(\mathcal{A}))\} e^{-itH(\mathcal{A})} \Psi_\alpha\|_{\mathcal{H}} \\
&\quad = (2\pi)^{-\frac{1}{2}} \| \int_{\mathbb{R}} d\sigma \hat{g}(\sigma) \{e^{i\sigma D/t} - e^{i\sigma 2H(\mathcal{A})}\} e^{-itH(\mathcal{A})} \Psi_\alpha \|_{\mathcal{H}} \\
&\quad \le (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} d\sigma (1+|\sigma|) \sup_{|s|\le S} \frac{1}{1+|s|} \|\{e^{isD/t} - e^{is2H(\mathcal{A})}\} e^{-itH(\mathcal{A})} \Psi_\alpha\|_{\mathcal{H}} \\
&\quad +2\|\Psi_\alpha\|(2\pi)^{-\frac{1}{2}} \int_{|\sigma|>S} d\sigma (1+|\sigma|) \hat{g}(\sigma) \\
&\quad = \epsilon + \text{const}\,(g) \sup_{|s|<S} \|(D/t - 2H(\mathcal{A})) e^{2isH(\mathcal{A})} e^{-itH(\mathcal{A})} \Psi_\alpha\|_{\mathcal{H}}
\end{aligned}$$

because $\hat{g}$ is a Schwartz function and S is chosen large enough. Now observe that

$$\begin{aligned}
|t|^{-1} \|D e^{-iH(\mathcal{A})(t-2s)} \Psi_\alpha - (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} e^{-iH(\mathcal{A})(t-2s)} (H(\mathcal{A}) - z)^2 \Psi_\alpha\|_{\mathcal{H}} \\
\le |t|^{-1} \|[D, (H(\mathcal{A}) - z)^{-1}]\|_{\mathcal{B}(\mathcal{H})} \cdot \|(H(\mathcal{A}) - z)^2 \Psi_\alpha\|_{\mathcal{H}},
\end{aligned}$$

which is less than ϵ for $|t| \ge T(\epsilon)$ uniformily in s, where $T(\epsilon)$ is an appropiately chosen constant. By using Lemma 7.4.1, one only needs to estimate the last of the latter terms:

$$\begin{aligned}
&t^{-1} e^{itH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} e^{-itH(\mathcal{A})} \\
&\quad = \; t^{-1} (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} \\
&\qquad + t^{-1} \int_0^1 \frac{d}{ds} e^{isH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} e^{-isH(\mathcal{A})} ds \\
&\quad = \; t^{-1} (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} \\
&\qquad + t^{-1} \int_0^1 e^{isH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} i[H(\mathcal{A}), D] (H(\mathcal{A}) - z)^{-1} e^{-isH(\mathcal{A})} ds \\
&\quad = \; t^{-1} (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} \\
&\qquad + t^{-1} \int_0^1 e^{isH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} (2H(\mathcal{A}) + k) (H(\mathcal{A}) - z)^{-1} e^{-isH(\mathcal{A})} ds \\
&\quad = \; t^{-1} (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} + 2H(\mathcal{A}) (H(\mathcal{A}) - z)^{-2} \\
&\qquad + t^{-1} \int_0^1 e^{isH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} k (H(\mathcal{A}) - z)^{-1} e^{-isH(\mathcal{A})} ds \\
&\quad = \; t^{-1} (H(\mathcal{A}) - z)^{-1} D (H(\mathcal{A}) - z)^{-1} \\
&\qquad + 2H(\mathcal{A}) (H(\mathcal{A}) - z)^{-2} + t^{-1} \int_0^1 e^{isH(\mathcal{A})} C e^{-isH(\mathcal{A})} ds,
\end{aligned}$$

where C is the operator such that $C = (H(\mathcal{A}) - z)^{-1} K (H(\mathcal{A}) - z)^{-1}$.

Hence, for $t \geq T(\epsilon)$, we have that

$$
\begin{aligned}
&\sup_{|s| \leq S} \|(D/t - 2H(\mathcal{A}))e^{-i(t-2s)H(\mathcal{A})}\Psi_\alpha\|_{\mathcal{H}} \\
&\qquad = \epsilon + |t|^{-1} \sup_{|s| \leq S} \|(H(\mathcal{A}) - z)^{-1} D e^{-2isH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} \Psi_\alpha\|_{\mathcal{H}} \\
&\qquad + \|t^{-1} \int_0^1 e^{isH(\mathcal{A})} C e^{-isH(\mathcal{A})} P_{\mathrm{c}}(H(\mathcal{A})) ds\|_{\mathcal{B}(\mathcal{H})} \cdot \|(H(\mathcal{A}) - z)^2 \Psi_\alpha\|_{\mathcal{H}} \\
&\qquad \|C\|_{\mathcal{B}(\mathcal{H})} \cdot \|(H(\mathcal{A}) - z)^2 P_p(H(\mathcal{A}))\Psi_\alpha\|_{\mathcal{H}}.
\end{aligned}
$$

The second term is estimated by

$$
\begin{aligned}
&\|(H(\mathcal{A}) - z)^{-1} [(\boldsymbol{p} - \mathcal{A}) \cdot \boldsymbol{x} + id/2] e^{2isH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} \Psi_\alpha\|_{\mathcal{H}} \\
&\quad \leq \|(H(\mathcal{A}) - z)^{-1} |\boldsymbol{p} - \mathcal{A}|\|_{\mathcal{B}(\mathcal{H})} \cdot \||\boldsymbol{x}| e^{-2isH(\mathcal{A})} (H(\mathcal{A}) - z)^{-1} \Psi\alpha\|_{\mathcal{H}} + id/2 \|\Psi\alpha\|_{\mathcal{H}}
\end{aligned}
$$

which is uniformly bounded on every compact s-interval, so for $|t|^{-1}$ large enough. The third term is tend to zero as $t \to \infty$ by RAGE Theorem 4.3.1. Finally, one can estimate the last term,

$$\|C\|_{\mathcal{B}(\mathcal{H})} \cdot \|(H(\mathcal{A}) - z)^2 P_p(H(\mathcal{A}))\Psi_\alpha\|_{\mathcal{H}} \leq \epsilon \|C\|_{\mathcal{B}(\mathcal{H})}.$$

□

As a consequence, we have:

Corollary 7.4.4 *Let Assumption 7.1.1 hold. Then*

1. For $\Psi \in \mathcal{H}_c(H(\mathcal{A}))$,

$$\lim_{|t| \to \infty} e^{-itH(\mathcal{A})}\Psi = 0.$$

2. For $g \in C_0^\infty(\mathbb{R})$ and $\Psi \in \mathcal{H}_c(H(\mathcal{A}))$ with $\Psi = g(H(\mathcal{A}))\Psi$,

$$\lim_{t \to \infty} \|e^{-itH(\mathcal{A})}\Psi - g(H_0) e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} = 0.$$

Proof. 1. The set of $\Psi \in \mathcal{H}_{\mathrm{c}}(H(\mathcal{A}))$ for which there exists a function $g \in C_0^\infty(\mathbb{R})$ with supp g such that $g(2H(\mathcal{A}))\Psi = \Psi$ is dense in $\mathcal{H}_{\mathrm{c}}(H(\mathcal{A}))$. Moreover,

$$s - \lim_{|t| \to \infty} g(D/t) = 0$$

For $\Phi \in \mathcal{H}$

$$\begin{aligned}
|\langle \Phi, e^{-itH(\mathcal{A})}\Psi\rangle_{\mathcal{H}}| &= |\langle \Phi, g(2H(\mathcal{A}))e^{-itH(\mathcal{A})}\Psi\rangle_{\mathcal{H}} + \langle \Phi, g(D/t) - g(D/t)\Psi\rangle_{\mathcal{H}}| \\
&= |\langle \Phi, \{g(2H(\mathcal{A})) - g(D/t)\}e^{-itH(\mathcal{A})}\Psi\rangle_{\mathcal{H}} + \langle \Phi, g(D/t)\Psi\rangle_{\mathcal{H}}| \\
&\leq \|\Phi\|_{\mathcal{H}} \cdot \|\{g(2H(\mathcal{A})) - g(D/t)\}e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} + \|g(D/t)\Phi\|_{\mathcal{H}} \cdot \|\Psi\|_{\mathcal{H}} \\
&\longrightarrow 0 \qquad \text{for} \qquad |t| \to \infty
\end{aligned}$$

2. Need to show that $e^{itH(\mathcal{A})}H_0 e^{-itH(\mathcal{A})}$ converges to $H(\mathcal{A})$ in the strong resolvent sense. Let $\Psi \in \mathcal{H}_{\mathrm{c}}(H(\mathcal{A}))$. Then

$$\begin{aligned}
&\|((H(\mathcal{A}) - z)^{-1} - (H_0 - z)^{-1})e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} \\
&= \|(H(\mathcal{A}) - z)^{-1}(H(\mathcal{A}) - H_0)(H_0 - z)^{-1}e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}} \\
&= |(H(\mathcal{A}) - z)^{-1}V_{\mathcal{A}}(H_0 - z)^{-1}e^{-itH(\mathcal{A})}\Psi\|_{\mathcal{H}}
\end{aligned}$$

$\square$

Propagation

Let $H(\mathcal{A})$, N and D be as above.

Lemma 7.4.5 *Let Assumption 7.1.1 hold, and let $H(\mathcal{A}), N$ and D as above. For $\Psi \in$* Dom (N). *Then the quadratic form*

$$e^{itH(\mathcal{A})}i[H(\mathcal{A}), \frac{m}{2}\boldsymbol{x}^2]e^{-itH(\mathcal{A})} = e^{itH(\mathcal{A})}De^{-itH(\mathcal{A})}$$

is defined termwise on Dom $(N) \times$ Dom (N) *and it can be extended to an essentially self-adjoint operator on* Dom (N).

Proof. On $C_0^\infty(\mathbb{R}^d, \mathbb{C})$ the commutator $i[H(\mathcal{A}), \frac{m}{2}\boldsymbol{x}^2] = D$. The operator D is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d, \mathbb{C})$, i.e.,

$$\{\Psi \in \mathcal{H} : (D \pm i)\Psi, \quad \Psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C})\}$$

is dense in $\mathcal{H}$. Since $e^{-itH(\mathcal{A})}$ Dom $(N) =$ Dom (N) forall $t \in \mathbb{R}$ and Dom $(N) \subseteq$ Dom (D), the operator

$$D_t = e^{itH(\mathcal{A})}De^{-itH(\mathcal{A})}$$

is symmetric on $\mathrm{Dom}\,(N)$ for all (fixed) $t \in \mathbb{R}$. Now one can see that D_t is essentially self-adjoint because

$$(D_t \pm i)\Phi = e^{itH(\mathcal{A})}(D \pm i)e^{-itH(\mathcal{A})}\Phi$$

Since D is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d, \mathbb{C})$, the set $e^{itH(\mathcal{A})}\,\mathrm{Ran}\,(D_t \pm i) \subseteq \mathrm{Ran}\,(D \pm i)$ is dense in $\mathcal{H}$ and D_t is essentially self-adjoint on $\mathrm{Dom}\,(N)$. $\square$

Proposition 7.4.6 *Let Assumption 7.1.1 hold. If $\epsilon > 0, \Psi_\alpha \in \mathcal{H}_c(H(\mathcal{A}))$ and $\Psi_\alpha \in \mathrm{Dom}\,(N)$ is a family of vectors satisfying Lemma 7.4.1, then for some $C > 0$,*

$$\limsup_{t>0} \|\{\frac{\boldsymbol{x}}{t} - \frac{\boldsymbol{p}}{m}\}e^{-itH(\mathcal{A})}\Psi_\alpha\|_{\mathcal{H}} \leq C\epsilon \tag{7.10}$$

Proof. We take the norm of

$$\{\frac{\boldsymbol{x}}{t} - \frac{\boldsymbol{p}}{m}\}e^{-itH}\Psi_\alpha$$

squared,

$$\begin{aligned}
&\|\{\frac{\boldsymbol{x}}{t} - \frac{\boldsymbol{p}}{m}\}e^{-itH(\mathcal{A})}\Psi_\alpha\|^2_{\mathcal{H}} \\
&= \langle\{\frac{\boldsymbol{x}}{t} - \frac{\boldsymbol{p}}{m}\}e^{-itH(\mathcal{A})}\Psi_\alpha, \{\frac{\boldsymbol{x}}{t} - \frac{\boldsymbol{p}}{m}\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi_\alpha, \{\frac{\boldsymbol{x}}{t} - \frac{\boldsymbol{p}}{m}\}^2 e^{-itH(\mathcal{A})}\Psi_\alpha\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi_\alpha, \{\frac{\boldsymbol{x}^2}{t^2} - \frac{\boldsymbol{x}}{t}\frac{\boldsymbol{p}}{m} - \frac{\boldsymbol{p}}{m}\frac{\boldsymbol{x}}{t} + \frac{\boldsymbol{p}^2}{m^2}\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi_\alpha, \{\frac{\boldsymbol{x}^2}{t^2} - \frac{t^{-1}}{m}[\boldsymbol{xp} + \boldsymbol{px}] + \frac{\boldsymbol{p}^2}{m}\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi_\alpha, \frac{2}{m}\{\frac{m}{2}\frac{\boldsymbol{x}^2}{t^2} - \frac{t^{-1}}{2}[\boldsymbol{xp} + \boldsymbol{px}] + \frac{\boldsymbol{p}^2}{2m}\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle \\
&= \frac{2}{m}\langle e^{-itH(\mathcal{A})}\Psi_\alpha, \{\frac{m}{2}(\frac{\boldsymbol{x}}{t})^2 - t^{-1}\boldsymbol{D} + H_0\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle
\end{aligned}$$

Then,

$$\frac{2}{m}\langle e^{-itH(\mathcal{A})}\Psi_\alpha, \{\frac{m}{2}(\frac{\boldsymbol{x}}{t})^2 - t^{-1}\boldsymbol{D} + H_0\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle \tag{7.11}$$

Using Lemma 7.4.5, the time derivative of the first summand is

$$\begin{aligned}
&\frac{d}{dt}\langle e^{-itH(\mathcal{A})}\Psi, \frac{m}{2}\boldsymbol{x}^2 e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \frac{d}{dt}\langle\Psi, e^{itH(\mathcal{A})}\frac{m}{2}\boldsymbol{x}^2 e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle\Psi, e^{itH(\mathcal{A})}i[H(\mathcal{A}), \frac{m}{2}\boldsymbol{x}^2]e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, i[H(\mathcal{A}), \frac{m}{2}\boldsymbol{x}^2]e^{-itH(\mathcal{A})}\Psi\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{m}{2} i[H(\mathcal{A}), \boldsymbol{x}^2] e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{m}{2} i[H(\mathcal{A})_{\mathcal{A}}, \boldsymbol{x}^2] e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{m}{2} i[H(\mathcal{A})_{\mathcal{A}}, \boldsymbol{x}^2] e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{m}{2} i[\frac{(\boldsymbol{p}-\mathcal{A})^2}{2m}, \boldsymbol{x}^2] e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{i}{4}\left([(\boldsymbol{p}-\mathcal{A}), \boldsymbol{x}^2](\boldsymbol{p}-\mathcal{A}) + (\boldsymbol{p}-\mathcal{A})[(\boldsymbol{p}-\mathcal{A}), \boldsymbol{x}^2]\right) e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{i}{4}\left((-2i\boldsymbol{x})(\boldsymbol{p}-\mathcal{A}) + (\boldsymbol{p}-\mathcal{A})(-2i\boldsymbol{x})\right) e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{1}{2}\left(\boldsymbol{x}\cdot(\boldsymbol{p}-\mathcal{A}) + (\boldsymbol{p}-\mathcal{A})\cdot\boldsymbol{x}\right) e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \frac{1}{2}\left(\boldsymbol{x}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{x}\right) e^{-itH(\mathcal{A})}\Psi\rangle \\
&= \langle e^{-itH(\mathcal{A})}\Psi, \boldsymbol{D} e^{-itH(\mathcal{A})}\Psi\rangle
\end{aligned}
$$

Where $H(\mathcal{A}) = H_{\mathcal{A}} + V$. We used that fact $\frac{m}{2} i[H_{\mathcal{A}}, \boldsymbol{x}^2] = D$ with

$$
D = \frac{1}{2}(\boldsymbol{x}\boldsymbol{p} + \boldsymbol{p}\boldsymbol{x}) \tag{7.12}
$$

Now

$$
\begin{aligned}
&t^{-2}\langle\Psi_\alpha, e^{itH(\mathcal{A})}\frac{m}{2}\boldsymbol{x}^2 e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\langle\Psi_\alpha, e^{itH(\mathcal{A})}\frac{m}{2}\boldsymbol{x}^2 e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} - t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\int_0^t ds \frac{d}{ds}\langle\Psi_\alpha, e^{isH(\mathcal{A})}\frac{m}{2}\boldsymbol{x}^2 e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\int_0^t ds \langle\Psi_\alpha, e^{isH(\mathcal{A})} i[H(\mathcal{A}), \frac{m}{2}\boldsymbol{x}^2] e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\int_0^t ds \langle\Psi_\alpha, e^{isH(\mathcal{A})}\{D\} e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\int_0^t ds \langle\Psi_\alpha, e^{isH(\mathcal{A})}\{D\} e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} + H(\mathcal{A}) - H(\mathcal{A}) \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\int_0^t ds\cdot s\langle\Psi_\alpha, e^{isH(\mathcal{A})}\{D/s - 2H(\mathcal{A})\} e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} + H(\mathcal{A})
\end{aligned}
$$

Now, we have

$$
\begin{aligned}
&\frac{2}{m}\langle e^{-itH(\mathcal{A})}\Psi_\alpha, e^{itH(\mathcal{A})}\{\frac{m}{2}(\frac{\boldsymbol{x}}{t})^2 - \frac{D}{t} + H_0\} e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\int_0^t ds\cdot s\langle\Psi_\alpha, e^{isH(\mathcal{A})}\{D/s - 2H(\mathcal{A})\} e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} \\
&\quad + \langle\Psi_\alpha, e^{itH(\mathcal{A})}\{-D/t - 2H(\mathcal{A}) + 2H(\mathcal{A})\} e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} + \\
&\quad \langle\Psi_\alpha, e^{itH(\mathcal{A})} H_0 e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}} + H(\mathcal{A}) \\
&= t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}} + t^{-2}\int_0^t ds\cdot s\langle\Psi_\alpha, e^{isH(\mathcal{A})}\{D/s - 2H(\mathcal{A})\} e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}}
\end{aligned}
$$

$$
\begin{aligned}
&+\langle\Psi_\alpha, e^{itH(\mathcal{A})}\{2H(\mathcal{A})-D/t\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}}\\
&+\langle\Psi_\alpha, e^{itH(\mathcal{A})}\{H_0+H(\mathcal{A})-2H(\mathcal{A})\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle\\
= \ &t^{-2}\langle\Psi_\alpha, \frac{m}{2}\boldsymbol{x}^2\Psi_\alpha\rangle_{\mathcal{H}}+t^{-2}\int_0^t ds\cdot s\langle\Psi_\alpha, e^{isH(\mathcal{A})}\{D/s-2H(\mathcal{A})\}e^{-isH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}}\\
&+\langle\Psi_\alpha, e^{itH(\mathcal{A})}\{2H(\mathcal{A})-D/t\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}}+\langle\Psi_\alpha, e^{itH(\mathcal{A})}\{H_0-H(\mathcal{A})\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle_{\mathcal{H}}
\end{aligned}
$$

The first term goes to zero. Second and third terms follow from the proof of Theorem 7.4.3, assertion 1.

$$
\limsup_{t\to\infty}\langle\Psi_\alpha, e^{itH(\mathcal{A})}\{D/t-2H(\mathcal{A})\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle\le K\|\Psi-\Psi_\alpha\|
$$

for large enough t. Here we estimate last term,

$$
\begin{aligned}
&\|\langle\Psi_\alpha, e^{itH(\mathcal{A})}\{H(\mathcal{A})-H_0\}e^{-itH(\mathcal{A})}\Psi_\alpha\rangle\|_{\mathcal{H}}\\
&\quad=\|\langle\Psi_\alpha, e^{itH(\mathcal{A})}Ve^{-itH(\mathcal{A})}\Psi_\alpha\rangle\|_{\mathcal{H}}\\
&\quad\le\|(H(\mathcal{A})-z)\Psi_\alpha\|_{\mathcal{H}}\cdot\|(H(\mathcal{A})-z)^{-1}V(H(\mathcal{A})-z)^{-1}e^{-itH(\mathcal{A})}P_c(H(\mathcal{A}))(H(\mathcal{A})-z)\Psi_\alpha\|_{\mathcal{H}}\\
&\quad+\|\Psi_\alpha\|_{\mathcal{H}}\cdot\|V_{\mathcal{A}}(H(\mathcal{A})-z)^{-1}\|_{\mathcal{B}(\mathcal{H})}\cdot\|(H(\mathcal{A})-z)P_P(H(\mathcal{A}))\Psi_\alpha\|_{\mathcal{H}}\\
&\quad\le K\|\Psi-\Psi_\alpha\|_{\mathcal{H}}
\end{aligned}
$$

Since $(H(\mathcal{A})-z)^{-1}V_{\mathcal{A}}(H(\mathcal{A})-z)^{-1}$ is compact and $e^{-itH(\mathcal{A})}P_c(H(\mathcal{A}))(H(\mathcal{A})-z)\Psi_\alpha$ converge weakly to zero, due to previous Theorem 7.4.3 (2). The last term is bounded by const. ϵ, provided α is chosen large enough. Notice that the constant in the last term is proportional to $\|\Psi_\alpha\|_{\mathcal{H}}$, because Ψ_α converge to Ψ as $\alpha\to\infty$, so $\|\Psi_\alpha\|_{\mathcal{H}}$ becomes a bounded .

□

We are now ready to establish the main theorem.

Proof of Theorem 1.0.3.

$$
\begin{aligned}
&\|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi\|_{\mathcal{H}}\\
&\quad=\ \|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi\|_{\mathcal{H}}-\|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi'\|_{\mathcal{H}}\\
&\quad\quad+\|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi'\|_{\mathcal{H}}\\
&\quad\le\ \|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}(\Psi-\Psi')\|_{\mathcal{H}}+\|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi'\|_{\mathcal{H}}\\
&\quad\le\ 2\|f\|_{L^\infty}\|\Psi-\Psi'\|_{\mathcal{H}}+\|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi'\|_{\mathcal{H}}
\end{aligned}
$$

Now we apply the BCH Formula (see Theorem A.4.1)

$$\begin{aligned} f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m}) &= \int_0^1 d\lambda\{(\nabla f)(\frac{\boldsymbol{x}}{t}+\lambda(\frac{\boldsymbol{p}}{m}-\frac{\boldsymbol{x}}{t})\cdot(\frac{\boldsymbol{x}}{t}-\frac{\boldsymbol{p}}{m})) \\ &+ \frac{1}{t}\frac{i}{2m}(\Delta f)(\frac{\boldsymbol{x}}{t}+\lambda(\frac{\boldsymbol{p}}{m}-\frac{\boldsymbol{x}}{t}))\} \end{aligned}$$

Since $\nabla f, \Delta f \in C_0^\infty(\mathbb{R}^\nu)$, so

$$\|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iHt}\Psi'\|_{\mathcal{H}} \leq C_1\|\{\frac{\boldsymbol{x}}{t}-\frac{\boldsymbol{p}}{m}\}e^{-itH(\mathcal{A})}\Psi'\|_{\mathcal{H}}+\frac{C_2}{t}$$

Now we will show that claim is a dense subset of $\mathcal{H}_c(H(\mathcal{A}))$, we assume that Ψ is in subset and so $\mathrm{Dom}\,(H_c) \subseteq \mathcal{H}_c(H(\mathcal{A}))$, and $\Psi' = (H(\mathcal{A})-z)^{-1}\Phi$ with $\Phi \in \mathrm{Dom}\,(N)$

$$\|\Psi-\Psi'\|_{\mathcal{H}} \leq \epsilon$$

and shows that

$$\limsup_{t>0}\|\{f(\frac{\boldsymbol{x}}{t})-f(\frac{\boldsymbol{p}}{m})\}e^{-iH(\mathcal{A})t}\Psi'\|_{\mathcal{H}} \leq C\epsilon$$

where C does not depends on Ψ', is a bounded function $C = C(\Psi')$ of Ψ', then the estimates holds. In view of Proposition 7.4.6 we have, for $\Psi_\alpha \in \mathrm{Dom}\,(N)$ is a real family of vector such that $\{\Psi_\alpha : \alpha > 0\}$, then thats properties satisfied

$$\begin{aligned} &\Psi_\alpha \in \mathrm{Dom}\,(N), \qquad \text{for all } \ \alpha > 0 \\ &\|\Psi-\Psi_\alpha\| \longrightarrow 0, \quad \alpha \to \infty \\ &\|(H(\mathcal{A})-z)P_p(H(\mathcal{A}))\Psi_\alpha\| \longrightarrow 0, \quad \alpha \to \infty \end{aligned}$$

□

Generalization

We assume that a transversal (Poincarè) gauge 7.1 exists and given by the formula

$$\mathcal{A}_n(\boldsymbol{x}) := \sum_{m=1}^{d}\int_0^1 \xi\mathcal{F}_{mn}(\xi\boldsymbol{x})\,d\xi\boldsymbol{x}_m \qquad n = 1, ..., d \tag{7.13}$$

where $\mathcal{F}_{mn}$ is the field strength (tensor). We thus begin by imposing condition on the physically relevant entities $\mathcal{F}_{mn}$ and div $\mathcal{A}$, where $\mathcal{A}(\boldsymbol{x}) = (\mathcal{A}_1(\boldsymbol{x}), ..., \mathcal{A}_d(\boldsymbol{x}))$.

Assumption 7.4.7 *Assume that*

i) div $\mathcal{A} \in L^2_{loc}(\mathbb{R}^\nu)$ *for* $d \leq 3$

ii) div $\mathcal{A} \in L^q_{loc}(\mathbb{R}^\nu)$ *for* $d \geq 3, d/2 \leq q \leq \infty,$ *and* $q > 2$

iii) div $\mathcal{A}$ *is* H_0*-bounded with relative bound less that 1.*

iv) Decay condition

$$\|\,\mathrm{div}\ \mathcal{A}(H_0+i)^{-1}\chi(|\boldsymbol{x}|>R)\|_{\mathcal{B}(\mathcal{H})} \in L^1(\mathbb{R}^+, dR) \tag{7.14}$$

$$\|\,\mathrm{div}\ \mathcal{A}\chi(|\boldsymbol{x}|>R)(H_0+i)^{-1}\|_{\mathcal{B}(\mathcal{H})} \in L^1(\mathbb{R}^+, dR) \tag{7.15}$$

The hypotheses on the field strength $\mathcal{F}_{mn}$ and $\sum_{m=1}^{d} \mathcal{F}_{mn}(\boldsymbol{x})x_n$ are summarized in the following where we set $\mathcal{F}_{mn} = \mathcal{F}^b_{mn} + \mathcal{F}^s_{mn}$, with $\mathcal{F}^b_{mn}$, resp, $\mathcal{F}^s_{mn}$ being associated with a bounded, resp. singular, pert of $\mathcal{F}_{mn}$.

Assumption 7.4.8 *i) For* $d \leq 3$ *and for some* $0 < \nu < 1$,

$$\mathcal{F}^b_{lm} \in L^\infty(\mathbb{R}^d) \quad \textit{with} \quad \left|\mathcal{F}^b_{lm}(\boldsymbol{x})\right| \leq c(1+|\boldsymbol{x}|)^{-(1+\nu)} \tag{7.16}$$

$$\mathcal{F}^s_{lm} \in L^4_{loc}(\mathbb{R}^d), \int_{B(0,r)} \left|\sum_{l=1}^{d} \mathcal{F}^s_{lm}(\boldsymbol{x})x_l\right|^4 d\boldsymbol{x} \leq c(r)^\mu \tag{7.17}$$

for $r > 0, \mu > d-1$

ii) For $d \geq 4, d \leq q \leq \infty,$ *and* $q > 4$ *and for some* $0 < \nu < 1$,

$$\mathcal{F}^s_{lm} \in L^q_{loc}(\mathbb{R}^d), \int_{B(0,r)} \left|\sum_{l=1}^{d} \mathcal{F}^s_{lm}(\boldsymbol{x})x_l\right|^q d\boldsymbol{x} \leq c(r)^\mu \tag{7.18}$$

for $r > 0, \mu > d-1$

iii)

$$\mathrm{supp}\ \mathcal{F}^s_{lm} \subset B(0,R_0) \ \textit{for}\ R_0 > 0 \tag{7.19}$$

iv) For $0 < \nu < 1$ *and* $u > \max\{2d, d/(1-\nu)\}$

$$\mathcal{F}^s_{lm} \in L^{loc}_u(\mathbb{R}^d) \tag{7.20}$$

Assumption 7.4.9 *Let Assumption 7.4.7 be satisfied. Then*

i) For $d \leq 3$

$$\mathcal{A}_n \in L^4_{loc}(\mathbb{R}^d) \tag{7.21}$$

ii) For $d \geq 4, d \leq q \leq \infty,$ and $q > 4$

$$\mathcal{A}_n \in L^q_{loc}(\mathbb{R}^d) \tag{7.22}$$

iii) $|\mathcal{A}_n(\boldsymbol{x})|^2$ and $\mathcal{A}_n(\boldsymbol{x})\boldsymbol{p}$ are H_0-bounded with relative bound less that 1.

iv)

$$\|\mathcal{A}_n(\boldsymbol{x})(H_0 + i1)^{-\frac{1}{2}}\|_{\mathcal{B}(\mathcal{H})} < \infty \tag{7.23}$$

v) Decay conditions : for $0 < \nu < 1$

$$\|\mathcal{A}_n(\boldsymbol{x})\chi(|\boldsymbol{x}| > R)(H_0 + i)^{-\frac{1}{2}}\|_{\mathcal{B}(\mathcal{H})} \leq cR^{-\nu} \tag{7.24}$$

$$\||\mathcal{A}_n(\boldsymbol{x})|^2\chi(|\boldsymbol{x}| > R)(H_0 + i)^{-1}\|_{\mathcal{B}(\mathcal{H})} \leq cR^{-2\nu} \tag{7.25}$$

Theorem 7.4.10 *Let Assumption 7.4.7 and 7.4.8 be satisfied. Then $H = (\boldsymbol{p} - \mathcal{A}(\boldsymbol{x}))^2$ is a self-adjoint operator on $\mathcal{H}$ with domain $\operatorname{Dom}(H) = \operatorname{Dom}(H_0) = \boldsymbol{H}^2(\mathbb{R}^d; \mathbb{C})$. Moreover, H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d; \mathbb{C})$.*

Lemma 7.4.11 *Let Assumption 7.4.7 and 7.4.8 be satisfied. Then*

1. $e^{-itH}\operatorname{Dom}(N) = \operatorname{Dom}(N)$ for all $t \in \mathbb{R}$

2. $\|(1 + |\boldsymbol{x}|)^\gamma e^{-itH}\Psi\|_{\mathcal{H}} \leq c(\Psi)(1 + |t|)^\gamma$ for $\gamma = 1, 2$ and $\Psi \in \operatorname{Dom}(N)$

3. There exists a $z \in \mathbb{C}, \operatorname{Im} z \neq 0,$ such that $(H - z)^{-1}\operatorname{Dom}(N) \subset \operatorname{Dom}(N)$

Lemma 7.4.12 *Let Assumption 7.4.7 and 7.4.8 be satisfied. Then the assertions of Lemma 7.3.1 and Lemma 7.4.5.*

Proof. We only give the necessary modifications. Assumptions 7.4.7 and Assumptions 7.4.8 imply that

$$\begin{aligned}
&\|H_0(H - z)^{-1}\|\mathcal{B}(\mathcal{H}) + \|H(H_0 - z)^{-1}\|_{\mathcal{B}(\mathcal{H})} < \infty \\
&\|\mathcal{A}\boldsymbol{p}(H - z)^{-1}\|\mathcal{B}(\mathcal{H}) + \|\mathcal{A}\boldsymbol{p}(H_0 - z)^{-1}\|_{\mathcal{B}(\mathcal{H})} < \infty \\
&\|\operatorname{div}\, \mathcal{A}(H - z)^{-1}\|\mathcal{B}(\mathcal{H}) + \|\operatorname{div}\, \mathcal{A}(H_0 - z)^{-1}\|_{\mathcal{B}(\mathcal{H})} < \infty \\
&\||\mathcal{A}|^2(H - z)^{-1}\|\mathcal{B}(\mathcal{H}) + \||\mathcal{A}|^2(H_0 - z)^{-1}\|_{\mathcal{B}(\mathcal{H})} < \infty
\end{aligned} \tag{7.26}$$

Bearing in mind $A_{\mathcal{A}}$ from proof of Lemma 7.3.1, Assumption (iv) 7.4.7 we infer that the difference

$$
\begin{aligned}
& (H_0 - z)^{-1} - (H - z)^{-1} && (7.27)\\
= \ & (H_0 - z)^{-1} V_{\mathcal{A}} (H - z)^{-1} && (7.28)\\
= \ & (H_0 - z)^{-1} (1 + |\boldsymbol{x}|)^{-1/2} (1 + |\boldsymbol{x}|)^{1/2} (H - z)^{-1} && (7.29)
\end{aligned}
$$

is compact; begin a product of a compact operator and a bounded one. Here we use that $f(\boldsymbol{x})(H_0 - \zeta)^{-1}$ is compact provided $f \in L^\infty(\mathbb{R}^d)$ tends to zero at infinity. Likewise, it follows from Assumption 7.4.7 (iv) and Assumption 7.4.9 that

$$
\begin{aligned}
& (H_0 - z)^{-1} (1 + |\boldsymbol{x}|) V_{\mathcal{A}} (H - z)^{-1} \\
= \ & (H_0 - z)^{-1/2} \chi(|\boldsymbol{x}| < R)(1 + |\boldsymbol{x}|) V_{\mathcal{A}} (H - z)^{-1} \\
& + (H_0 - z)^{-1/2} \chi(|\boldsymbol{x}| < R)(1 + |\boldsymbol{x}|) V_{\mathcal{A}} (H - z)^{-1} \qquad (7.30)
\end{aligned}
$$

is a compact because its a sum of compact operators for any R and an operator with arbitrary small norm. Having summarized these consequences of our hypothesis, we follow the proof of Lemma 7.3.1. By Lemma 7.26 $(H_0 - z)^{1/2} \mathcal{A} \boldsymbol{p} (H - z)^{-1}$ and its adjoint is bounded. By our hypotheses and the consequences (7.26) -(7.26) all operators like div $\mathcal{A}(H - z)^{-1}, (H - z)^{-1} V_{\mathcal{A}} (H - z)^{-1}$ and $(H_0 - z)^{-1/2}(1 + |\boldsymbol{x}|) V_{\mathcal{A}} (H - z)^{-1}$ and their adjoints are compact. Thus the operator C, defined in Lemma 7.3.1, is compact. □

It is easy to see from the proof of Lemma 7.4.1 that it holds under the assumptions in ref. and relative H_0-boundedness with relative bound less than one. Hence:

Lemma 7.4.13 *Let Assumption 7.4.7 (i-iii) and 7.4.8 (i-iii) be satisfied. Then the assertion of Lemma 7.4.1 are valid.*

As a consequence, we have:

Theorem 7.4.14 *Let Assumption 7.4.7 and 7.4.8 be satisfied. Then Theorem 1.0.3 hold.*

Appendix A

Auxiliary results

A.1 Hörmander's method of non-stationary phase

Theorem A.1.1 *Let K be a compact subset of $\mathbb{R}^d$ with interior K^{int}, and let ϕ be a real-valued function in $C^{k+1}(\Omega)$, where Ω is an open neighborhood of K. Suppose that $\nabla\phi \neq 0$ on K. Then, for any $u \in C_0^k(K^{int})$ and $\omega \in \mathbb{R}$.*

$$\left| \int e^{i\omega\phi(y)} u(y)\, dy \right| \leq C_k |\omega|^{-k} \|u\|_{k,\infty}$$

where C_k depends on K and ϕ and

$$\|u\|_{k,\infty} = \sum_{|\alpha|\leq k} \sup |(d^\alpha u)(y)|$$

If $\mathcal{V} \subset C^{k+1}(\Omega)$ is a family of function satisfying

(i) $|\nabla\phi| > C > 0$ on K for all $\phi \in \mathcal{V}$

(ii) $\sum_{2\leq\alpha<K+1} \sup_{y\in K} |(\partial^\alpha\phi)(y)| < M < \infty$ for some M and all $\phi \in \mathcal{V}$ then the constant C_k can be chosen uniform in $\phi \in \mathcal{V}$.

A.2 Commutator theorem

A self-adjoint operator $N \geq 1$ on a Hilbert space $\mathcal{H}$ generates a scale of Hilbert spaces $\mathcal{H}_n$, $n = 0, \pm1, \pm2, \ldots$, which arise as the closure of $\mathrm{Dom}\,(N^{\frac{n}{2}})$ with respect to the norm $\|\cdot\|_{\mathcal{H}_n} := \|N^{\frac{n}{2}} \cdot\|_{\mathcal{H}}$. The scale has the following properties:

1. For every integer n: $\mathcal{H}_{n+1} \subseteq \mathcal{H}_n$, $\|\cdot\|_{\mathcal{H}_n} \leq \|\cdot\|_{\mathcal{H}_{n+1}}$.

2. For all $m \geq n$, $\mathcal{H}_m$ is dense in $\mathcal{H}_n$ with respect to $\|\cdot\|_{\mathcal{H}_n}$.

3. The operator $N^{\frac{n}{2}} : \mathcal{H}_m \to \mathcal{H}_{m-n}$ is unitary for all m and n.

4. For every integer n, the space $\mathcal{H}_n^*$ is conjugate isometrically isomorphic to $\mathcal{H}_{-n}$.

5. $\mathcal{H}_\infty \equiv \cap_{n=0}^{\infty} \mathcal{H}_n$ is dense in $\mathcal{H}$.

Glimm-Jaffe [15] and Nelson [22] established the following result; see also [11].

Theorem A.2.1 (Commutator Theorem) *Let $N \geq 1$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Assume $A \in \mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ is a symmetric operator and that $[N, A] \in \mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$. Then:*

1. The operator $\widetilde{A}$ associated to A is densely defined in $\mathcal{H}$.

2.[1] $\mathrm{Dom}\,(N) \subseteq \mathrm{Dom}\,(\widetilde{A})$ *and, for all* $\Psi \in \mathrm{Dom}\,(N)$,

$$\|\widetilde{A}\Psi\|_{\mathcal{H}} \leq c\,\|N\Psi\|_{\mathcal{H}}.$$

3. The operator $\widetilde{A}$ is essentially self-adjoint on every core of N.

A.3 Invariant domains

If $A \in \mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ is a symmetric operator and the commutator $[N, A]$ belongs to $\mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$, then the operator $\widetilde{A}$ associated to A is densely defined and essentially self-adjoint on $\mathrm{Dom}\,(N) \subseteq \mathrm{Dom}\,(\widetilde{A})$ and, moreover, $\widetilde{A}$ is relatively bounded with respect to N. Therefore the one-parameter group $\exp(it\widetilde{A})$ is well-defined. The aim of this section is to investigate how the group $\exp(it\widetilde{A})$ acts on the domains of $N^{\frac{1}{2}}$ and N. Fröhlich established the following result [13]. As therein it is convenient to denote $i[N, A]$ by $\dot{A}$.

Theorem A.3.1 *Suppose that $A \in \mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ is symmetric and that $\dot{A} \in \mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$. Then $\exp(it\widetilde{A})$ is well-defined and, in addition,*

1. $\exp(it\widetilde{A})\mathfrak{Q}(N) \subseteq \mathfrak{Q}(N)$ *and, for all* $\Psi \in \mathfrak{Q}(N)$,

$$\|N^{\frac{1}{2}} e^{it\widetilde{A}}\Psi\|_{\mathcal{H}} \leq e^{c_1|t|}\|N^{\frac{1}{2}}\Psi\|_{\mathcal{H}}.$$

2. $\exp(it\widetilde{A})\,\mathrm{Dom}\,(N) \subseteq \mathrm{Dom}\,(N)$ *and, for all* $\Psi \in \mathrm{Dom}\,(N)$,

$$\|N e^{it\widetilde{A}}\Psi\|_{\mathcal{H}} \leq e^{c_2|t|}\|\Psi\|_{\mathcal{H}}.$$

3. $\exp(it\widetilde{A})\,\mathrm{Dom}\,(N^{\beta}) = \mathrm{Dom}\,(N^{\alpha})$ *for* $\alpha = 1/2, 1$.

[1] Since $N \geq 1$, this means that $\widetilde{A}$ is relatively bounded with respect to N.

A.4 Baker-Campbell-Hausdorff theorem

Theorem A.4.1 (Baker-Campbell-Hausdorff) *If $\beta \in \mathbb{R}$ and $g \in C^2_\infty(\mathbb{R}^d)$, the set of twice continuously differentiable functions for which all the derivatives tend to zero at infinity, then the Baker-Campbell-Hausdorff formula holds:*

$$g(\beta \boldsymbol{p}) - g(\boldsymbol{x}) = \int_0^1 \Big\{ (\nabla g)(\boldsymbol{x} + \lambda(\beta \boldsymbol{p} - \boldsymbol{x})) \cdot (\beta \boldsymbol{p} - \boldsymbol{x}) \quad - i\frac{\beta}{2}(\Delta g)(\boldsymbol{x} + \lambda(\beta \boldsymbol{p} - \boldsymbol{x})) \Big\}\, d\lambda.$$

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