


Summer 7-29-2017

Trace formulas for perturbations of operators with Hilbert-Schmidt resolvents

Bishnu Prasad Sedai
University of New Mexico

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Bishnu Prasad Sedai

Candidate

Mathematics and Statistics

Department

This dissertation is approved, and it is acceptable in quality and form for publication:

Approved by the Dissertation Committee:

Anna Skripka, Chairperson

Maria Cristina Pereyra

Maxim Zinchenko

Andres A. Contreras Marcillo

**TRACE FORMULAS FOR PERTURBATIONS OF OPERATORS
WITH HILBERT-SCHMIDT RESOLVENTS**

BY

BISHNU PRASAD SEDAI

M.A., Mathematics, Tribhuvan University, 2004

DISSERTATION

Submitted in Partial Fulfillment of the
Requirements for the Degree of
Doctor of Philosophy

Mathematics

The University of New Mexico
Albuquerque, New Mexico

July, 2017

Acknowledgments

First of all, I would like to express my sincere gratitude to my advisor, Anna Skripka, who has been eminently supportive during the last three years to explain the concepts and to let me grow in this fascinating area of mathematics at my own pace. Without her guidance and persistent help this dissertation would not have been possible.

I am extremely grateful to my family and friends for their support and encouragement throughout my graduate school years.

With great pleasure, I would like to thank Anna Skripka and Matthew Blair for their NSF grant support.

Finally, many thanks to all my other dissertation committee members: Maria Cristina Pereyra, Maxim Zinchenko, and Andres A. Contreras Marcillo.

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Abstract

In this dissertation, we study Taylor approximations of functions of operators with Hilbert-Schmidt resolvents. We obtain integral representations for traces of the respective Taylor remainders that are analogous to trace formulas obtained in the case of Schatten perturbations in [10, 11, 16].

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Chapter 1

Introduction

Let H_0 be a closed densely defined self-adjoint operator (for simplicity we will just write “self-adjoint” in the sequel), V a bounded self-adjoint operator on a separable Hilbert space \mathcal{H} , f a sufficiently nice function, and let $f(H_0)$ and $f(H_0 + V)$ be defined by the functional calculus. Consider the remainder of the Taylor approximation

$$R_{n,H_0,V}(f) := f(H_0 + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV),$$

where $n \in \mathbb{N}$ and the Gâteaux derivatives $\frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV)$ are evaluated in the uniform operator topology. If a self-adjoint perturbation V is in the Schatten-von Neumann ideal of compact operators \mathcal{S}^n , then the following trace formula holds:

$$\mathrm{Tr}(R_{n,H_0,V}(f)) = \int_{\mathbb{R}} f^{(n)}(t) \eta_n(t) dt, \quad (1.0.1)$$

where $\eta_n = \eta_{n,H_0,V}$ is a real valued L^1 -function depending only on H_0 and V . The history of representation (1.0.1) started in physics in the late 40’s and the first mathematical result was proved by M. G. Krein for $n = 1$ in 1953 [11]. The results for $n = 2$ and $n \geq 3$ were established by L. S. Koplienko in 1984 [10] and by D. Potapov, A. Skripka, and F. Sukochev in 2013 [16], respectively. If the perturbations of the operators are not compact and no additional restriction on the initial operator H_0 is imposed, then the trace of $R_{n,H_0,V}(f)$ is usually undefined. Noncompact perturbations mainly arise in the study of differential operators because they are multiplications by functions defined on \mathbb{R}^d , which are not compact operators. In this case, the condition that the perturbations are in some Schatten-von Neumann ideal of the compact operators \mathcal{S}^n gets replaced by the restriction on the resolvent of the initial (unperturbed) operators.

In this dissertation, we prove trace formulas similar to (1.0.1) under different assumptions on H_0 , V , and f . We assume that the resolvent of H_0 belongs to \mathcal{S}^2 , V is a bounded self-adjoint linear operator on \mathcal{H} , and $f \in C_c^n((a, b))$, where $C_c^n((a, b))$ is the space of n times continuously differentiable functions on \mathbb{R} that are compactly supported in $(a, b) \subset \mathbb{R}$. We show that there exists a unique locally finite real-valued measure $\mu_n = \mu_{n, H_0, V}$, $n \geq 3$, such that the following trace formula holds:

$$\mathrm{Tr}(R_{n, H_0, V}(f)) = \int_{\mathbb{R}} f^{(n)}(t) d\mu_n(t). \quad (1.0.2)$$

In the special case of commuting H_0 and V , we show that the measure μ_n in (1.0.2) is absolutely continuous, so that there exists a locally integrable function $\eta_n = \eta_{n, H_0, V}$, $n \geq 3$, such that the trace formula (1.0.1) holds. The formula (1.0.1) with locally integrable η_n for $n = 1$ and $n = 2$ was proved in [2, Theorem 2.5] and [18, Theorem 3.10], respectively.

This work is divided mainly into two chapters. In Chapter 2, we derive formulas for the derivatives of operator functions. Derivatives of operator functions can be written as multiple operator integrals (see, e.g., [3]). We give an example of the multiple operator integral representing a derivative of a finite dimensional matrix function. We also show that derivatives of more general operator functions can be expressed via Bochner integrals. Although it is a known result, we prove it here by straightforward calculations and use it to prove our central results. In particular, we use it to prove (1.0.1) in the commutative case.

Chapter 3 is devoted to the main results of this dissertation and we follow [18] to prove our results. We divide Chapter 3 into two sections. In the first section, we consider the general case and prove the formula (1.0.2). In the second section, we consider the commutative case and prove the formula (1.0.1). We also give examples of a Hilbert space and operators to which the formulas (1.0.1) and (1.0.2) apply.

The Appendix collects standard definitions and facts about operators, spectral theory, Bochner integrals, the Schwartz class functions, and the Fourier transform that are applied in the dissertation.

In this work, \mathcal{H} denotes a separable complex Hilbert space, $\mathcal{B}(\mathcal{H})$ the space of all bounded linear operators on \mathcal{H} , H_0 a self-adjoint operator in \mathcal{H} , and Tr denotes the standard trace. The symbol $E_{H_0}(\cdot)$ stands for the spectral measure of a self-adjoint operator H_0 . As usually, $\sigma(H_0)$ and $\rho(H_0)$ denote the spectrum and resolvent set of H_0 , respectively.

Chapter 2

Calculation of operator derivatives

The formulas for derivatives of operator functions derived in this chapter are well known, but they appeared in the literature without a detailed calculation. Moreover, our calculation of these derivatives is straightforward and does not appeal to the most general theory of differentiation of operator functions, which can be found in, for example, [3].

2.1 Divided differences

The formulas for operator derivatives involve the object known under the names divided difference or difference quotient. The definition and basic properties of the divided difference are given in this section; for more comprehensive treatment of this object we refer the reader to [8, Section 4.7].

Definition 2.1.1. *Let $n \in \mathbb{N}$. The divided difference of order n is an operation on functions $f \in C^n(\mathbb{R})$ of one (real) variable, which we usually call λ , defined recursively as follows:*

$$\begin{aligned} f^{[0]}[\lambda_1] &:= f(\lambda_1), \\ f^{[n]}[\lambda_1, \dots, \lambda_{n-1}, \lambda_n, \lambda_{n+1}] &:= \begin{cases} \frac{f^{[n-1]}[\lambda_1, \dots, \lambda_{n-1}, \lambda_n] - f^{[n-1]}[\lambda_1, \dots, \lambda_{n-1}, \lambda_{n+1}]}{\lambda_{n-1} - \lambda_n} & \text{if } \lambda_n \neq \lambda_{n+1} \\ \left. \frac{\partial}{\partial t} \right|_{t=\lambda_{n+1}} f^{[n-1]}[\lambda_1, \dots, \lambda_{n-1}, t] & \text{if } \lambda_n = \lambda_{n+1}. \end{cases} \end{aligned}$$

The following two lemmas are simple properties of divided differences that we use later in the proof of Theorem 2.2.7 below.

Lemma 2.1.2. *Let $f(\lambda) := \lambda^n$ for $n \in \mathbb{N}$. Then,*

$$f^{[p]}[\lambda_1, \lambda_2, \dots, \lambda_{p+1}] = \sum_{\substack{0 \leq n_0, n_1, \dots, n_p \\ n_0 + n_1 + \dots + n_p = n-p}} \lambda_1^{n_0} \lambda_2^{n_1} \dots \lambda_{p+1}^{n_p}, \quad p \leq n.$$

Proof. The lemma can be proved by induction on p . Here, we give the proof only for $p = 2$. Note that $f^{[2]}[\lambda_1, \lambda_2, \lambda_3] = f^{[2]}[\lambda_{\sigma(1)}, \lambda_{\sigma(2)}, \lambda_{\sigma(3)}]$, where σ is a permutation on $\{1, 2, 3\}$, and $f^{[1]}[\lambda_1, \lambda_2] = f^{[1]}[\lambda_2, \lambda_1]$. We consider the following three different cases:

Case (1): $\lambda_1 \neq \lambda_2 \neq \lambda_3$.

By Definition 2.1.1,

$$\begin{aligned} & f^{[2]}[\lambda_1, \lambda_2, \lambda_3] \\ &= \frac{f^{[1]}[\lambda_2, \lambda_3] - f^{[1]}[\lambda_1, \lambda_2]}{\lambda_3 - \lambda_1} \\ &= \frac{\frac{f(\lambda_3) - f(\lambda_2)}{\lambda_3 - \lambda_2} - \frac{f(\lambda_2) - f(\lambda_1)}{\lambda_2 - \lambda_1}}{\lambda_3 - \lambda_1} \\ &= \frac{\frac{\lambda_3^n - \lambda_2^n}{\lambda_3 - \lambda_2} - \frac{\lambda_2^n - \lambda_1^n}{\lambda_2 - \lambda_1}}{\lambda_3 - \lambda_1} \\ &= \frac{\lambda_3^{n-1} + \lambda_3^{n-2}\lambda_2 + \dots + \lambda_3\lambda_2^{n-2} + \lambda_2^{n-1} - \lambda_2^{n-1} - \lambda_2^{n-2}\lambda_1 - \dots - \lambda_2\lambda_1^{n-2} - \lambda_1^{n-1}}{\lambda_3 - \lambda_1} \\ &= \frac{(\lambda_3^{n-1} - \lambda_1^{n-1}) + \lambda_2(\lambda_3^{n-2} - \lambda_1^{n-2}) + \lambda_2^2(\lambda_3^{n-3} - \lambda_1^{n-3}) + \dots + \lambda_2^{n-2}(\lambda_3 - \lambda_1)}{\lambda_3 - \lambda_1} \\ &= \frac{(\lambda_3 - \lambda_1) \left[\sum_{i=0}^{n-2} \lambda_3^i \lambda_1^{n-2-i} + \lambda_2 \sum_{i=0}^{n-3} \lambda_3^i \lambda_1^{n-3-i} + \dots + \lambda_2^{n-3}(\lambda_3 + \lambda_1) + \lambda_2^{n-2} \right]}{(\lambda_3 - \lambda_1)} \\ &= \sum_{m=1}^{n-1} \sum_{i=0}^{m-1} \lambda_3^i \lambda_1^{m-1-i} \lambda_2^{n-1-m}. \end{aligned}$$

Since $0 \leq i, (m-1-i), (n-1-m)$ and $i + (m-1-i) + (n-1-m) = n-2$, we have

$$f^{[2]}[\lambda_1, \lambda_2, \lambda_3] = \sum_{\substack{0 \leq n_0, n_1, n_2 \\ n_0 + n_1 + n_2 = n-2}} \lambda_1^{n_0} \lambda_2^{n_1} \lambda_3^{n_2}.$$

Case (2): $\lambda_1 = \lambda_2 \neq \lambda_3$.

By Definition 2.1.1,

$$f^{[2]}[\lambda_1, \lambda_1, \lambda_3] = \frac{f^{[1]}[\lambda_1, \lambda_3] - f^{[1]}[\lambda_1, \lambda_1]}{\lambda_3 - \lambda_1}$$

$$\begin{aligned}
& \frac{f(\lambda_3) - f(\lambda_1)}{\lambda_3 - \lambda_1} - f'(\lambda_1) \\
= & \frac{\frac{\lambda_3^n - \lambda_1^n}{\lambda_3 - \lambda_1} - n\lambda_1^{n-1}}{\lambda_3 - \lambda_1} \\
= & \frac{\lambda_3^{n-1} + \lambda_3^{n-2}\lambda_1 + \dots + \lambda_3\lambda_1^{n-2} + \lambda_1^{n-1} - n\lambda_1^{n-1}}{\lambda_3 - \lambda_1} \\
= & \frac{(\lambda_3^{n-1} - \lambda_1^{n-1}) + \lambda_1(\lambda_3^{n-2} - \lambda_1^{n-2}) + \lambda_1^2(\lambda_3^{n-3} - \lambda_1^{n-3}) + \dots + \lambda_1^{n-2}(\lambda_3 - \lambda_1)}{\lambda_3 - \lambda_1} \\
= & \frac{(\lambda_3 - \lambda_1) \left[\sum_{i=0}^{n-2} \lambda_3^i \lambda_1^{n-2-i} + \lambda_1 \sum_{i=0}^{n-3} \lambda_3^i \lambda_1^{n-3-i} + \dots + \lambda_1^{n-3}(\lambda_3 + \lambda_1) + \lambda_1^{n-2} \right]}{(\lambda_3 - \lambda_1)} \\
= & \sum_{m=1}^{n-1} \sum_{i=0}^{m-1} \lambda_3^i \lambda_1^{m-1-i} \lambda_1^{n-1-m}.
\end{aligned}$$

Since $0 \leq i, (m-1-i), (n-1-m)$ and $i + (m-1-i) + (n-1-m) = n-2$,

$$f^{[2]}[\lambda_1, \lambda_1, \lambda_3] = \sum_{\substack{0 \leq n_0, n_1, n_2 \\ n_0 + n_1 + n_2 = n-2}} \lambda_1^{n_0} \lambda_1^{n_1} \lambda_3^{n_2}.$$

Using the symmetry of divided difference and proceeding as in case(2), we can prove the cases $\lambda_1 = \lambda_3 \neq \lambda_2$ and $\lambda_2 = \lambda_3 \neq \lambda_1$.

Case (3): $\lambda_1 = \lambda_2 = \lambda_3$.

By Definition 2.1.1,

$$\begin{aligned}
f^{[2]}[\lambda_1, \lambda_1, \lambda_1] &= \frac{f''(\lambda_1)}{2!} \\
&= \frac{n(n-1)}{2} \lambda_1^{n-2} \\
&= \frac{n-1}{2} \{2(1) + (n-2)(1)\} \lambda_1^{n-2} \\
&= [(n-1) + (n-2) + \dots + 3 + 2 + 1] \lambda_1^{n-2} \\
&= (n-1)\lambda_1^{n-2} + (n-2)\lambda_1^{n-2} + \dots + 3\lambda_1^{n-2} + 2\lambda_1^{n-2} + \lambda_1^{n-2} \\
&= \sum_{i=0}^{n-2} \lambda_1^i \lambda_1^{n-2-i} + \lambda_1 \sum_{i=0}^{n-3} \lambda_1^i \lambda_1^{n-3-i} + \dots + \lambda_1^{n-3}(\lambda_1 + \lambda_1) + \lambda_1^{n-2} \\
&= \sum_{m=1}^{n-1} \sum_{i=0}^{m-1} \lambda_1^i \lambda_1^{m-1-i} \lambda_1^{n-1-m}.
\end{aligned}$$

Since $0 \leq i, (m-1-i), (n-1-m)$ and $i + (m-1-i) + (n-1-m) = n-2$,

we have

$$f^{[2]}[\lambda_1, \lambda_1, \lambda_1] = \sum_{\substack{0 \leq n_0, n_1, n_2 \\ n_0 + n_1 + n_2 = n-2}} \lambda_1^{n_0} \lambda_1^{n_1} \lambda_1^{n_2}.$$

□

Lemma 2.1.3. $(f + g)^{[n]}[\lambda_0, \lambda_1, \dots, \lambda_n] = f^{[n]}[\lambda_0, \lambda_1, \dots, \lambda_n] + g^{[n]}[\lambda_0, \lambda_1, \dots, \lambda_n]$, where $f, g \in C^n(\mathbb{R})$.

2.2 Derivatives of operator functions

In this section, we calculate the derivatives of operator rational functions and operator functions with nice Fourier transforms.

2.2.1 Basic differentiation rules

In this section, we define Gâteaux derivative and discuss some basic rules for it.

Definition 2.2.1. Let U be a closed densely defined self-adjoint operator in \mathcal{H} and $V = V^* \in \mathcal{B}(\mathcal{H})$. Let $f : \mathbb{R} \mapsto \mathbb{C}$ be a bounded function. Then, the Gâteaux derivative of the mapping $U \rightarrow f(U)$ at U in the direction V is defined by

$$\left. \frac{d}{ds} \right|_{s=0} f(U + sV) = \lim_{s \rightarrow 0} \frac{f(U + sV) - f(U)}{s},$$

if the limit exists in the operator norm (uniform operator topology).

The following two lemmas are the sum and product rules for Gâteaux derivatives.

Lemma 2.2.2. Let U be a closed densely defined self-adjoint operator in \mathcal{H} and $V = V^* \in \mathcal{B}(\mathcal{H})$. Let $f, g : \mathbb{R} \mapsto \mathbb{C}$ be bounded functions such that the mappings $U \rightarrow f(U)$ and $U \rightarrow g(U)$ are Gâteaux differentiable at U in the direction V . Then, the mapping $U \rightarrow (f + g)(U)$ is also Gâteaux differentiable at U in the direction V and

$$\left. \frac{d}{dt} \right|_{t=0} (f + g)(U + tV) = \left. \frac{d}{dt} \right|_{t=0} f(U + tV) + \left. \frac{d}{dt} \right|_{t=0} g(U + tV).$$

Proof. By Definition 2.2.1,

$$\begin{aligned} \left. \frac{d}{dt} \right|_{t=0} (f + g)(U + tV) &= \lim_{t \rightarrow 0} \frac{(f + g)(U + tV) - (f + g)(U)}{t} \\ &= \lim_{t \rightarrow 0} \frac{f(U + tV) + g(U + tV) - f(U) - g(U)}{t} \\ &= \lim_{t \rightarrow 0} \left[\frac{f(U + tV) - f(U)}{t} + \frac{g(U + tV) - g(U)}{t} \right]. \end{aligned}$$

Now, we have

$$\begin{aligned} & \left\| \frac{f(U + tV) - f(U)}{t} + \frac{g(U + tV) - g(U)}{t} - \left(\frac{d}{dt} \Big|_{t=0} f(U + tV) + \frac{d}{dt} \Big|_{t=0} g(U + tV) \right) \right\| \\ & \leq \left\| \frac{f(U + tV) - f(U)}{t} - \frac{d}{dt} \Big|_{t=0} f(U + tV) \right\| + \\ & \quad \left\| \frac{g(U + tV) - g(U)}{t} - \frac{d}{dt} \Big|_{t=0} g(U + tV) \right\| \rightarrow 0 \end{aligned}$$

as $|t| \rightarrow 0$ since both the mappings $U \rightarrow f(U)$ and $U \rightarrow g(U)$ are Gâteaux differentiable at U in the direction V . Therefore,

$$\lim_{t \rightarrow 0} \left[\frac{f(U + tV) - f(U)}{t} + \frac{g(U + tV) - g(U)}{t} \right] = \frac{d}{dt} \Big|_{t=0} f(U + tV) + \frac{d}{dt} \Big|_{t=0} g(U + tV)$$

and which completes the proof. \square

Lemma 2.2.3. *Let U be a closed densely defined self-adjoint operator in \mathcal{H} and $V = V^* \in \mathcal{B}(\mathcal{H})$. Let $f, g : \mathbb{R} \mapsto \mathbb{C}$ be bounded functions such that the mappings $U \rightarrow f(U)$ and $U \rightarrow g(U)$ are Gâteaux differentiable at U in the direction V . Then, the mapping $U \rightarrow (fg)(U)$ is also Gâteaux differentiable at U in the direction V and*

$$\frac{d}{dt} \Big|_{t=0} (fg)(U + tV) = \frac{d}{dt} \Big|_{t=0} f(U + tV)g(U) + f(U) \frac{d}{dt} \Big|_{t=0} g(U + tV).$$

Proof. The proof is similar to that of Lemma 2.2.2. \square

2.2.2 Derivatives of operator rational functions

A polynomial of an operator is defined only if the operator is bounded. The rational function $f(t) = (t - z)^{-k}$, $z \in \mathbb{C} \setminus \mathbb{R}$, $k \in \mathbb{N}$ is bounded and continuous on \mathbb{R} so that we can define $f(U)$ as a bounded operator even if $U = U^*$ is an unbounded operator.

The case of a finite dimensional Hilbert space

In this section, we collect technical facts on derivatives of operator polynomial functions.

Lemma 2.2.4. *Let \mathcal{H} be a finite dimensional Hilbert space and let $U, V \in \mathcal{B}(\mathcal{H})$. Let $f(x) := x^n$, $n \in \mathbb{N}$. Then,*

$$\frac{d}{ds} \Big|_{s=t} f(U + sV) = \sum_{j=0}^{n-1} (U + tV)^j V (U + tV)^{n-j-1},$$

where the limits are evaluated in the uniform operator topology.

Proof. The proof directly follows from Definition 2.2.1 and the fact that

$$\left. \frac{d}{ds} \right|_{s=t} f(U + sV) = \left. \frac{d}{ds} \right|_{s=0} f(U + (s+t)V).$$

□

Remark 2.2.5. *The above lemma is still true if we consider \mathcal{H} to be an infinite dimensional Hilbert space and follows as in the case of finite dimensional Hilbert space.*

Lemma 2.2.6. *Let \mathcal{H} be an m dimensional Hilbert space and $U = U^*$ be an $m \times m$ matrix on \mathcal{H} . Then,*

$$U^k = \sum_{i=1}^m \lambda_i^k E_i,$$

where $k \in \mathbb{N}$, $\{\lambda_i\}_{i=1}^m$ are eigenvalues of U counting multiplicity, and $E_i : \mathcal{H} \mapsto \mathcal{H}$ is the spectral projection corresponding to the eigenvalue λ_i .

Proof. Let $\{e_i\}_{i=1}^m$ be an orthonormal basis of eigenvectors such that $Ue_i = \lambda_i e_i$. Then every $x \in \mathcal{H}$ has a unique representation

$$x = \sum_{i=1}^m \alpha_i e_i,$$

where $\alpha_i = \langle x, e_i \rangle = x^T \bar{e}_i$.

Since $Ue_i = \lambda_i e_i$ and U is linear, we have

$$Ux = \sum_{i=1}^m \lambda_i \alpha_i e_i.$$

Since E_i is the spectral projection in \mathcal{H} onto the $\text{span}\{e_i\}$, $E_i(x) = \alpha_i e_i$. Therefore, the last expression becomes

$$Ux = \sum_{i=1}^m \lambda_i E_i(x) \text{ for every } x \in \mathcal{H}.$$

Hence, we get the following representation for U :

$$U = \sum_{i=1}^m \lambda_i E_i.$$

By the just obtained result,

$$U^2 = \left(\sum_{i=1}^m \lambda_i E_i \right) \left(\sum_{j=1}^m \lambda_j E_j \right)$$

$$= \sum_{i=1}^m \lambda_i^2 E_i \quad \text{since } E_i E_j = \begin{cases} E_i & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}.$$

Assume that

$$U^k = \sum_{i=1}^m \lambda_i^k E_i.$$

Then,

$$\begin{aligned} U^{k+1} &= U^k U = \left(\sum_{i=1}^m \lambda_i^k E_i \right) \left(\sum_{j=1}^m \lambda_j E_j \right) \\ &= \sum_{i=1}^m \lambda_i^{k+1} E_i \quad \text{since } E_i E_j = \begin{cases} E_i & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}. \end{aligned}$$

Therefore by induction,

$$U^k = \sum_{i=1}^m \lambda_i^k E_i,$$

for all k . □

A derivative of an operator function can be written as a multiple operator integral (see, e.g., [3, Theorem 5.7]). The multiple operator integral representing a derivative of a finite dimensional matrix function has a simpler formula, an example of which we provide below. In the derivation of the following result, we adjust the proof of [7, Theorem 1] for the first order derivative of a matrix polynomial.

Theorem 2.2.7. *Let \mathcal{H} be an m dimensional Hilbert space. Let $U = U^* \in \mathcal{B}(\mathcal{H})$ and $V \in \mathcal{B}(\mathcal{H})$. Let f be a polynomial of degree n . Then,*

$$\begin{aligned} & \left. \frac{d^p}{dt^p} \right|_{t=0} f(U + tV) \\ &= p! \sum_{i_1=1}^m \sum_{i_2=1}^m \dots \sum_{i_{p+1}=1}^m f^{[p]}[\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_{p+1}}] E_{i_1} V E_{i_2} V \dots V E_{i_{p+1}}, \quad p \leq n, \end{aligned}$$

where $\{\lambda_i\}_{i=1}^m$ is the spectrum of U counting multiplicity, $f^{[p]}[\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_{p+1}}]$ is the divided difference of order p , and $E_i : \mathcal{H} \mapsto \mathcal{H}$ is the spectral projection corresponding to the eigenvalue λ_i .

Proof. The theorem can be proved by induction on p . Here, we give the proof only for $p = 1, 2$. Let us take $\mathcal{H} = \mathbb{C}^m$, $U = U^*$ and V to be $m \times m$ matrices on \mathcal{H} . We

prove the theorem for a monomial $f(x) = x^k$, $k \in \mathbb{N}$, and the application of Lemma 2.1.3 and Lemma 2.2.2 will give the result for a general polynomial function of the form

$f(x) = \alpha_n x^n + \alpha_{n-1} x^{n-1} + \dots + \alpha_3 x^3 + \alpha_2 x^2 + \alpha_1 x + \alpha_0$. By Lemma 2.2.4,

$$\left. \frac{d}{dt} \right|_{t=0} (U + tV)^k = \sum_{j=0}^{k-1} U^j V U^{k-j-1}.$$

By Lemma 2.2.6, the last expression becomes

$$\begin{aligned} \left. \frac{d}{dt} \right|_{t=0} (U + tV)^k &= \sum_{j=0}^{k-1} \sum_{i_1=1}^m \lambda_{i_1}^j E_{i_1} V \sum_{i_2=1}^m \lambda_{i_2}^{k-j-1} E_{i_2} \\ &= \sum_{i_1=1}^m \sum_{i_2=1}^m \sum_{j=0}^{k-1} \lambda_{i_1}^j \lambda_{i_2}^{k-j-1} E_{i_1} V E_{i_2}. \end{aligned} \quad (2.2.1)$$

Since

$$\sum_{j=0}^{k-1} \lambda_{i_1}^j \lambda_{i_2}^{k-j-1} = \begin{cases} \frac{\lambda_{i_1}^k - \lambda_{i_2}^k}{\lambda_{i_1} - \lambda_{i_2}} & \text{if } \lambda_{i_1} \neq \lambda_{i_2} \\ k \lambda_{i_1}^{k-1} & \text{if } \lambda_{i_1} = \lambda_{i_2} \end{cases}$$

and using Definition 2.1.1, the equation (2.2.1) becomes

$$\left. \frac{d}{dt} \right|_{t=0} (U + tV)^k = \sum_{i_1=1}^m \sum_{i_2=1}^m f^{[1]}[\lambda_{i_1}, \lambda_{i_2}] E_{i_1} V E_{i_2},$$

which proves the theorem for $p = 1$.

Next, we prove the theorem for $p = 2$. By the definition of second order operator derivative,

$$\left. \frac{d^2}{dt^2} \right|_{t=0} (U + tV)^k = \lim_{t \rightarrow 0} \frac{\left. \frac{d}{ds} \right|_{s=t} (U + sV)^k - \left. \frac{d}{ds} \right|_{s=0} (U + sV)^k}{t},$$

where the limit is evaluated in the uniform operator topology. By Lemma 2.2.4, the above expression becomes

$$\begin{aligned} \left. \frac{d^2}{dt^2} \right|_{t=0} (U + tV)^k &= \lim_{t \rightarrow 0} \frac{\sum_{j=0}^{k-1} (U + tV)^j V (U + tV)^{k-j-1} - \sum_{j=0}^{k-1} U^j V U^{k-j-1}}{t} \\ &= \sum_{j=0}^{k-1} \lim_{t \rightarrow 0} \frac{(U + tV)^j V (U + tV)^{k-j-1} - U^j V U^{k-j-1}}{t}. \end{aligned}$$

By Lemma 2.2.3, we get

$$\begin{aligned} \frac{d^2}{dt^2} \Big|_{t=0} (U + tV)^k &= \sum_{j=0}^{k-1} \left(\frac{d}{dt} \Big|_{t=0} (U + tV)^j V U^{k-j-1} + U^j V \frac{d}{dt} \Big|_{t=0} (U + tV)^{k-j-1} \right) \\ &= \sum_{j=1}^{k-1} \frac{d}{dt} \Big|_{t=0} (U + tV)^j V U^{k-j-1} + \sum_{j=0}^{k-2} U^j V \frac{d}{dt} \Big|_{t=0} (U + tV)^{k-j-1}. \end{aligned}$$

Again by Lemma 2.2.4, the last expression equals

$$\begin{aligned} &\sum_{j=1}^{k-1} \left[\left(\sum_{i=0}^{j-1} U^i V U^{j-1-i} \right) V U^{k-j-1} \right] + \sum_{j=0}^{k-2} \left[U^j V \left(\sum_{i=0}^{k-j-2} U^i V U^{k-j-2-i} \right) \right] \\ &= \sum_{j=1}^{k-1} \sum_{i=0}^{j-1} U^i V U^{j-1-i} V U^{k-j-1} + \sum_{j=1}^{k-1} \sum_{i=0}^{k-j-1} U^{j-1} V U^i V U^{k-j-1-i} \\ &= \sum_{j=1}^{k-1} \left[\sum_{i=0}^{j-1} U^i V U^{j-1-i} V U^{k-j-1} + \sum_{i=0}^{k-j-1} U^{j-1} V U^i V U^{k-j-1-i} \right]. \end{aligned}$$

Since $0 \leq i$, $(j-1-i)$, $(k-j-1)$ and $i + (j-1-i) + (k-j-1) = k-2$;
 $0 \leq (j-1)$, i , $(k-j-1-i)$ and $(j-1) + i + (k-j-1-i) = k-2$,

$$\frac{d^2}{dt^2} \Big|_{t=0} (U + tV)^k = 2! \sum_{\substack{0 \leq n_0, n_1, n_2 \\ n_0 + n_1 + n_2 = k-2}} U^{n_0} V U^{n_1} V U^{n_2}. \quad (2.2.2)$$

Using Lemma 2.2.6, the equation (2.2.2) becomes

$$\begin{aligned} \frac{d^2}{dt^2} \Big|_{t=0} (U + tV)^k &= 2! \sum_{\substack{0 \leq n_0, n_1, n_2 \\ n_0 + n_1 + n_2 = k-2}} \sum_{i_1=1}^m \lambda_{i_1}^{n_0} E_{i_1} V \sum_{i_2=1}^m \lambda_{i_2}^{n_1} E_{i_2} V \sum_{i_3=1}^m \lambda_{i_3}^{n_2} E_{i_3} \\ &= 2! \sum_{i_1=1}^m \sum_{i_2=1}^m \sum_{i_3=1}^m \sum_{\substack{0 \leq n_0, n_1, n_2 \\ n_0 + n_1 + n_2 = k-2}} \lambda_{i_1}^{n_0} \lambda_{i_2}^{n_1} \lambda_{i_3}^{n_2} E_{i_1} V E_{i_2} V E_{i_3}. \end{aligned}$$

By Lemma 2.1.2, we get

$$\frac{d^2}{dt^2} \Big|_{t=0} (U + tV)^k = 2! \sum_{i_1=1}^m \sum_{i_2=1}^m \sum_{i_3=1}^m f^{[2]}[\lambda_{i_1}, \lambda_{i_2}, \lambda_{i_3}] E_{i_1} V E_{i_2} V E_{i_3}.$$

□

The case of an infinite dimensional Hilbert space

The following lemma will be used to prove Theorem 2.2.9 below.

Lemma 2.2.8. *Let $U = U^*$ be an operator in \mathcal{H} and $V = V^* \in \mathcal{B}(\mathcal{H})$. Let $t \in \mathbb{R}$ and $z \in \mathbb{C} \setminus \mathbb{R}$. Then,*

$$\lim_{t \rightarrow 0} (U + tV - zI)^{-1} = (U - zI)^{-1},$$

where the limit is evaluated in the uniform operator topology.

Proof. Since U and $U + tV$ are self-adjoint, the spectra of both U and $U + tV$ are subsets of \mathbb{R} . Hence for all $z \in \mathbb{C} \setminus \mathbb{R}$, the resolvent operators $(U - zI)^{-1}$ of U and $(U + tV - zI)^{-1}$ of $U + tV$ exist and are bounded on \mathcal{H} . By the spectral theorem (see [Appendix, Theorem 4.3.8]),

$$U + tV = \int_{\mathbb{R}} \lambda dE(\lambda),$$

where E is the spectral measure of $U + tV$ on \mathcal{H} defined on the σ -algebra of Borel subsets of \mathbb{R} and the convergence of the integral is understood in the strong operator topology. Since $f(\lambda) = \frac{1}{\lambda - z}$ is a bounded continuous function on \mathbb{R} , by the functional calculus (see [Appendix, Section 4.3.5]),

$$f(U + tV) = \int_{\mathbb{R}} f(\lambda) dE(\lambda).$$

Since $f(U + tV) = (U + tV - zI)^{-1}$, the last expression becomes

$$(U + tV - zI)^{-1} = \int_{\mathbb{R}} \frac{1}{\lambda - z} dE(\lambda).$$

By the well known result in functional calculus (see [Appendix, Theorem 4.3.6]),

$$\|(U + tV - zI)^{-1}\| = \left\| \int_{\mathbb{R}} \frac{1}{\lambda - z} dE(\lambda) \right\| \leq \sup_{\lambda \in \mathbb{R}} \frac{1}{|\lambda - z|}.$$

If $z = a + ib$, where $a, b \in \mathbb{R}$, then the last estimate becomes

$$\|(U + tV - zI)^{-1}\| \leq \sup_{\lambda \in \mathbb{R}} \frac{1}{|(\lambda - a) - ib|} = \sup_{\lambda \in \mathbb{R}} \frac{1}{((\lambda - a)^2 + b^2)^{\frac{1}{2}}} \leq \frac{1}{|b|}$$

By the just obtained estimate, we get

$$\begin{aligned} & \|(U + tV - zI)^{-1} - (U - zI)^{-1}\| \\ &= \|(U + tV - zI)^{-1} \left((U - zI) - (U + tV - zI) \right) (U - zI)^{-1}\| \\ &\leq \|(U + tV - zI)^{-1}\| |t| \|V\| \|(U - zI)^{-1}\| \\ &\leq \frac{1}{|b|} |t| \|V\| \|(U - zI)^{-1}\| \rightarrow 0 \end{aligned}$$

as $|t| \rightarrow 0$.

□

Theorem 2.2.9. Let $U = U^*$ be an operator in \mathcal{H} and $V = V^* \in \mathcal{B}(\mathcal{H})$. Let $t \in \mathbb{R}$ and $z \in \mathbb{C} \setminus \mathbb{R}$. Then,

$$\begin{aligned} & \left. \frac{d^p}{dt^p} \right|_{t=0} (U + tV - zI)^{-k} \\ &= (-1)^p p! \sum_{\substack{1 \leq k_0, k_1, \dots, k_p \leq k \\ k_0 + k_1 + \dots + k_p = k+p}} (U - zI)^{-k_0} V (U - zI)^{-k_1} V \dots V (U - zI)^{-k_p}. \end{aligned}$$

Proof. The theorem can be proved by induction on p for an arbitrary k . Here, we prove the theorem for $p = 1$ and $p = 2$ and only for $k = 1$ and $k = 2$.

Let $k = 1$.

By the definition of first order operator derivative,

$$\left. \frac{d}{dt} \right|_{t=0} (U + tV - zI)^{-1} = \lim_{t \rightarrow 0} \frac{(U + tV - zI)^{-1} - (U - zI)^{-1}}{t},$$

where the limit is evaluated in the uniform operator topology. The above expression can be rewritten as

$$\begin{aligned} & \left. \frac{d}{dt} \right|_{t=0} (U + tV - zI)^{-1} \\ &= \lim_{t \rightarrow 0} \frac{(U + tV - zI)^{-1} \left((U - zI) - (U + tV - zI) \right) (U - zI)^{-1}}{t} \\ &= - \lim_{t \rightarrow 0} \frac{(U + tV - zI)^{-1} tV (U - zI)^{-1}}{t} \\ &= - \lim_{t \rightarrow 0} (U + tV - zI)^{-1} V (U - zI)^{-1}. \end{aligned}$$

By Lemma 2.2.8, the last expression becomes

$$\begin{aligned} \left. \frac{d}{dt} \right|_{t=0} (U + tV - zI)^{-1} &= -(U - zI)^{-1} V (U - zI)^{-1} \\ &= - \sum_{\substack{1 \leq k_0, k_1 \leq 1 \\ k_0 + k_1 = 2}} (U - zI)^{-k_0} V (U - zI)^{-k_1}. \end{aligned} \tag{2.2.3}$$

Let $k = 2$.

By the definition of first order operator derivative,

$$\begin{aligned} & \left. \frac{d}{dt} \right|_{t=0} (U + tV - zI)^{-2} \\ &= \lim_{t \rightarrow 0} \frac{(U + tV - zI)^{-2} - (U - zI)^{-2}}{t} \\ &= \lim_{t \rightarrow 0} \frac{(U + tV - zI)^{-1} (U + tV - zI)^{-1} - (U - zI)^{-1} (U - zI)^{-1}}{t}, \end{aligned}$$

where the limit is evaluated in the uniform operator topology. By Lemma 2.2.3 applied to $f(U+tV) = (U+tV-zI)^{-1}$ and $g(U+tV) = (U+tV-zI)^{-1}$ and using (2.2.3), we get

$$\begin{aligned} & \left. \frac{d}{dt} \right|_{t=0} (U+tV-zI)^{-2} \\ &= -(U-zI)^{-1}V(U-zI)^{-1}(U-zI)^{-1} - (U-zI)^{-1}(U-zI)^{-1}V(U-zI)^{-1}. \end{aligned}$$

The above expression can be rewritten as

$$\begin{aligned} & \left. \frac{d}{dt} \right|_{t=0} (U+tV-zI)^{-2} \\ &= -\left[(U-zI)^{-1}V(U-zI)^{-2} + (U-zI)^{-2}V(U-zI)^{-1} \right]. \quad (2.2.4) \\ &= -\sum_{\substack{1 \leq k_0, k_1 \leq 2 \\ k_0+k_1=3}} (U-zI)^{-k_0}V(U-zI)^{-k_1}. \end{aligned}$$

Continuing this way, we can show that it is true for all k .

Next, we prove the theorem for $p = 2$.

Let $k = 1$.

As in the equality (2.2.3), we can show that

$$\left. \frac{d}{ds} \right|_{s=t} (U+sV-zI)^{-1} = -(U+tV-zI)^{-1}V(U+tV-zI)^{-1}. \quad (2.2.5)$$

By the definition of second order operator derivative,

$$\left. \frac{d^2}{dt^2} \right|_{t=0} (U+tV-zI)^{-1} = \lim_{t \rightarrow 0} \frac{\left. \frac{d}{ds} \right|_{s=t} (U+sV-zI)^{-1} - \left. \frac{d}{ds} \right|_{s=0} (U+sV-zI)^{-1}}{t},$$

where the limit is evaluated in the uniform operator topology. By (2.2.3), (2.2.5), and Lemma 2.2.3 applied to $f(U+tV) = (U+tV-zI)^{-1}V$ and $g(U+tV) = (U+tV-zI)^{-1}$, the last expression equals

$$\begin{aligned} & \left. \frac{d^2}{dt^2} \right|_{t=0} (U+tV-zI)^{-1} \\ &= -\lim_{t \rightarrow 0} \frac{(U+tV-zI)^{-1}V(U+tV-zI)^{-1} - (U-zI)^{-1}V(U-zI)^{-1}}{t} \\ &= -\left[-(U-zI)^{-1}V(U-zI)^{-1}V(U-zI)^{-1} \right. \\ & \quad \left. - (U-zI)^{-1}V(U-zI)^{-1}V(U-zI)^{-1} \right] \\ &= 2! (U-zI)^{-1}V(U-zI)^{-1}V(U-zI)^{-1} \\ &= 2! \sum_{\substack{1 \leq k_0, k_1, k_2 \leq 1 \\ k_0+k_1+k_2=3}} (U-zI)^{-k_0}V(U-zI)^{-k_1}V(U-zI)^{-k_2}. \end{aligned}$$

Let $k = 2$.

As in the equality (2.2.4), we can show that

$$\begin{aligned} & \left. \frac{d}{ds} \right|_{s=t} (U + sV - zI)^{-2} \\ &= - \left[(U + tV - zI)^{-1} V (U + tV - zI)^{-2} + (U + tV - zI)^{-2} V (U + tV - zI)^{-1} \right]. \end{aligned} \quad (2.2.6)$$

By the definition of second order operator derivative,

$$\left. \frac{d^2}{dt^2} \right|_{t=0} (U + tV - zI)^{-2} = \lim_{t \rightarrow 0} \frac{\left. \frac{d}{ds} \right|_{s=t} (U + sV - zI)^{-2} - \left. \frac{d}{ds} \right|_{s=0} (U + sV - zI)^{-2}}{t},$$

where the limit is evaluated in the uniform operator topology. By (2.2.4) and (2.2.6), the latter expression becomes

$$\begin{aligned} & \left. \frac{d^2}{dt^2} \right|_{t=0} (U + tV - zI)^{-2} \\ &= - \left[\lim_{t \rightarrow 0} \frac{(U + tV - zI)^{-1} V (U + tV - zI)^{-2} - (U - zI)^{-1} V (U - zI)^{-2}}{t} \right. \\ & \quad \left. + \lim_{t \rightarrow 0} \frac{(U + tV - zI)^{-2} V (U + tV - zI)^{-1} - (U - zI)^{-2} V (U - zI)^{-1}}{t} \right]. \end{aligned}$$

By Lemma 2.2.3 applied once to $f(U+tV) = (U+tV-zI)^{-1}V$ and $g(U+tV) = (U+tV-zI)^{-2}$ and next to $f(U+tV) = (U+tV-zI)^{-2}V$ and $g(U+tV) = (U+tV-zI)^{-1}$ and using (2.2.3) and (2.2.4), we get

$$\begin{aligned} & \left. \frac{d^2}{dt^2} \right|_{t=0} (U + tV - zI)^{-2} \\ &= - \left[-(U - zI)^{-1} V (U - zI)^{-1} V (U - zI)^{-2} \right. \\ & \quad - (U - zI)^{-1} V \left((U - zI)^{-1} V (U - zI)^{-2} + (U - zI)^{-2} V (U - zI)^{-1} \right) \\ & \quad - \left((U - zI)^{-1} V (U - zI)^{-2} V + (U - zI)^{-2} V (U - zI)^{-1} V \right) (U - zI)^{-1} \\ & \quad \left. - (U - zI)^{-2} V \left((U - zI)^{-1} V (U - zI)^{-1} \right) \right] \\ &= 2 \left[(U - zI)^{-1} V (U - zI)^{-1} V (U - zI)^{-2} + (U - zI)^{-1} V (U - zI)^{-2} V (U - zI)^{-1} \right. \\ & \quad \left. + (U - zI)^{-2} V (U - zI)^{-1} V (U - zI)^{-1} \right] \\ &= 2! \sum_{\substack{1 \leq k_0, k_1, k_2 \leq 2 \\ k_0 + k_1 + k_2 = 4}} (U - zI)^{-k_0} V (U - zI)^{-k_1} V (U - zI)^{-k_2}. \end{aligned}$$

Continuing this way, we can show that it is true for all k . □

2.2.3 Derivatives of operator functions with nice Fourier transforms

Derivatives of more general operator functions can be expressed via Bochner integrals, whose detailed discussion can be found in, for example, [Appendix, Section 4.4] and [19, Section V.5].

Formulas for operator derivatives

The main result is in Theorem 2.2.14. We will prove several auxiliary lemmas before the main result.

Lemma 2.2.10. *(Duhamel's formula)(See [3, Lemma 5.2]) If B is a self-adjoint operator in \mathcal{H} , if $V = V^* \in \mathcal{B}(\mathcal{H})$ and if $A = B + V$, then*

$$e^{isA} - e^{isB} = \int_0^s e^{i(s-t)A} i(A - B) e^{itB} dt, \quad s \in \mathbb{R},$$

where the integral is a Bochner integral and its convergence is understood in the strong operator topology. Moreover, if B is bounded, then the integral can be evaluated in the uniform operator topology.

Lemma 2.2.11. *Let $H_0 = H_0^*$ be an operator in \mathcal{H} and $V = V^* \in \mathcal{B}(\mathcal{H})$. Then,*

$$\lim_{t \rightarrow 0} e^{i\lambda(H_0 + tV)} = e^{i\lambda H_0}, \quad \lambda \in \mathbb{R},$$

where the limit is evaluated in the strong operator topology. Moreover, if H_0 is bounded, then the limit can be evaluated in the uniform operator topology.

Proof. Using Lemma 2.2.10 and by [Appendix, Theorem 4.3.6 (7)], we have

$$\begin{aligned} & \|e^{i\lambda(H_0 + tV)} - e^{i\lambda H_0}\| \\ &= \left\| \int_0^\lambda e^{i(\lambda-y)(H_0 + tV)} i t V e^{iy H_0} dy \right\| \\ &\leq \int_0^\lambda \|e^{i(\lambda-y)(H_0 + tV)} i t V e^{iy H_0}\| dy \\ &\leq |t| \|V\| \int_0^\lambda dy \\ &= |t| \|V\| \cdot \lambda \rightarrow 0, \quad \text{as } |t| \rightarrow 0. \end{aligned}$$

□

In the proof of the following lemmas, we will use basic properties of the Fourier transform, which can be found in [Appendix, Section 4.5.2].

Lemma 2.2.12. *Let $H_0 = H_0^*$ be an operator in \mathcal{H} and let f be such that $f, \hat{f} \in L^1(\mathbb{R})$. For $x \in \mathcal{H}$, the function $t \mapsto \hat{f}(t)e^{iH_0t}x$ from \mathbb{R} to \mathcal{H} is Bochner integrable, that is, there exists a sequence of simple functions $\{s_n^{H_0, x}\}$ which converges to $t \mapsto \hat{f}(t)e^{iH_0t}x$ almost everywhere and*

$$\int_{\mathbb{R}} \hat{f}(t)e^{iH_0t}x dt = \lim_{n \rightarrow \infty} \int_{\mathbb{R}} s_n^{H_0, x}(t) dt \quad (2.2.7)$$

in \mathcal{H} . Moreover, if H_0 is bounded, then the integral can be evaluated in the uniform operator topology.

Proof. By the well known result in functional calculus (see [Appendix, Theorem 4.3.6 (7)]),

$$\|e^{iH_0t}\| = \left\| \int_{\mathbb{R}} e^{i\lambda t} dE(\lambda) \right\| \leq \sup_{\lambda \in \mathbb{R}} |e^{i\lambda t}| = 1, \text{ for all } t \in \mathbb{R}. \quad (2.2.8)$$

By the estimate (2.2.8) and the formula for the Fourier transform of f (see [Appendix, Definition 4.5.2]), we have

$$\begin{aligned} \|\hat{f}(t)e^{iH_0t}\| &\leq |\hat{f}(t)| \|e^{iH_0t}\| \leq |\hat{f}(t)| = \frac{1}{\sqrt{2\pi}} \left| \int_{\mathbb{R}} f(\lambda) e^{-i\lambda t} d\lambda \right| \leq \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} |f(\lambda)| d\lambda \\ &< \infty, \end{aligned}$$

and which implies that $\hat{f}(t)e^{iH_0t} \in \mathcal{B}(\mathcal{H})$ for each $t \in \mathbb{R}$. We first show that the function $t \mapsto \hat{f}(t)e^{iH_0t}x$ is continuous.

By the standard properties of spectral integral (see [Appendix, Theorem 4.3.6 (6)]), for $x \in \mathcal{H}$, we have

$$\begin{aligned} \|\hat{f}(t)e^{iH_0t}x - \hat{f}(t_0)e^{iH_0t_0}x\|^2 &= \left\| \int_{\mathbb{R}} (\hat{f}(t)e^{i\lambda t} - \hat{f}(t_0)e^{i\lambda t_0}) d(E(\lambda)x) \right\|^2 \\ &= \int_{\mathbb{R}} \left| \hat{f}(t)e^{i\lambda t} - \hat{f}(t_0)e^{i\lambda t_0} \right|^2 d\langle E(\lambda)x, x \rangle, \quad t, t_0 \in \mathbb{R}, \end{aligned} \quad (2.2.9)$$

where E is the spectral measure of H_0 and $\langle E(\cdot)x, x \rangle$ is a finite scalar measure defined on the σ -algebra of Borel subsets of \mathbb{R} . Since $f \in L^1(\mathbb{R})$, \hat{f} is continuous on \mathbb{R} (see [Appendix, Proposition 4.5.4]). Also, for each $\lambda \in \mathbb{R}$, $e^{i\lambda t}$ is a continuous function of t in \mathbb{R} . Therefore, $\hat{f}(t)e^{i\lambda t}$ is a continuous function of t in \mathbb{R} for each $\lambda \in \mathbb{R}$ and, for each $\lambda \in \mathbb{R}$, we have

$$\lim_{t \rightarrow t_0} \left| \hat{f}(t)e^{i\lambda t} - \hat{f}(t_0)e^{i\lambda t_0} \right|^2 = 0, \quad t, t_0 \in \mathbb{R}. \quad (2.2.10)$$

Since $f \in L^1(\mathbb{R})$, \hat{f} is bounded on \mathbb{R} . So, there exists $M > 0$ such that

$$|\hat{f}(t)| \leq M \text{ for all } t \in \mathbb{R}.$$

Using the last estimate, we have

$$\left| \hat{f}(t)e^{i\lambda t} - \hat{f}(t_0)e^{i\lambda t_0} \right|^2 \leq 4M^2, \quad t, t_0 \in \mathbb{R}.$$

Since $\langle E(\cdot)x, x \rangle$ is a finite measure on \mathbb{R} , we also have

$$\int_{\mathbb{R}} 4M^2 d\langle E(\lambda)x, x \rangle < \infty.$$

Therefore, by the Lebesgue dominated convergence theorem and (2.2.10), we get

$$\lim_{t \rightarrow t_0} \int_{\mathbb{R}} \left| \hat{f}(t)e^{i\lambda t} - \hat{f}(t_0)e^{i\lambda t_0} \right|^2 d\langle E(\lambda)x, x \rangle = \int_{\mathbb{R}} 0 d\langle E(\lambda)x, x \rangle = 0. \quad (2.2.11)$$

From (2.2.9) and (2.2.11), we have

$$\lim_{t \rightarrow t_0} \|\hat{f}(t)e^{iH_0 t} x - \hat{f}(t_0)e^{iH_0 t_0} x\|^2 = 0.$$

Since $t_0 \in \mathbb{R}$ was arbitrary, the function $t \mapsto \hat{f}(t)e^{iH_0 t} x$ is continuous. For any $\alpha \in \mathcal{H}^*$, the function $t \mapsto \alpha(\hat{f}(t)e^{iH_0 t} x)$ is continuous from \mathbb{R} to \mathbb{C} , and hence, measurable. Moreover, $\{\hat{f}(t)e^{iH_0 t} x : t \in \mathbb{R}\} \subset \mathcal{H}$ is separable. By ([Appendix, Definition 4.4.2]), the function $t \mapsto \hat{f}(t)e^{iH_0 t} x$ is separably-valued. Therefore, the function $t \mapsto \hat{f}(t)e^{iH_0 t} x$ is measurable (see [Appendix, Theorem 4.4.3]). Also, since $\int_{\mathbb{R}} \|\hat{f}(t)e^{iH_0 t} x\| dt < \infty$, by [Appendix, Theorem 4.4.5], $t \mapsto \hat{f}(t)e^{iH_0 t} x$ is Bochner integrable. By [Appendix, Definition 4.4.4], there exists a sequence of simple functions $\{s_n^{H_0, x}\}$ that satisfies the assertions of the theorem.

If H_0 is bounded, then $t \mapsto \hat{f}(t)e^{iH_0 t}$ is continuous in the uniform operator topology. By an argument similar to the one above, we can show that the limit in (2.2.7) exists in the uniform operator topology. \square

Lemma 2.2.13. *Let $H_0 = H_0^*$ be an operator in a Hilbert space \mathcal{H} and let f be such that $f, \hat{f} \in L^1(\mathbb{R})$. Then,*

$$f(H_0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t)e^{iH_0 t} dt,$$

where the integral on the right is a Bochner integral and its convergence is evaluated in the strong operator topology. Moreover, if H_0 is bounded, then the integral can be evaluated in the uniform operator topology.

Proof. By the spectral theorem (see [Appendix, Theorem 4.3.8]),

$$H_0 = \int_{\mathbb{R}} \lambda dE(\lambda),$$

where E is the spectral measure of H_0 on \mathcal{H} defined on the σ -algebra of Borel subsets of \mathbb{R} and the convergence of the integral is understood in the strong operator topology. Since f is a bounded continuous function on \mathbb{R} , by [Appendix, Section 4.3.5], we have

$$f(H_0) = \int_{\mathbb{R}} f(\lambda) dE(\lambda).$$

By [Appendix, Theorem 4.3.6 (5)], we also have

$$\langle f(H_0)x, y \rangle = \int_{\mathbb{R}} f(\lambda) dw(\lambda), \quad x, y \in \mathcal{H}, \quad (2.2.12)$$

where $w(\cdot) = \langle E(\cdot)x, y \rangle$ is a finite scalar measure defined on the σ -algebra of Borel subsets of \mathbb{R} . Since $f, \hat{f} \in L^1(\mathbb{R})$, by the Fourier inversion formula, $f(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{i\lambda t} dt$. Therefore, the equation (2.2.12) becomes

$$\langle f(H_0)x, y \rangle = \int_{\mathbb{R}} \left(\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{i\lambda t} dt \right) dw(\lambda). \quad (2.2.13)$$

Since $|e^{i\lambda t}| = 1$,

$$\int_{\mathbb{R}} \left(\int_{\mathbb{R}} |\hat{f}(t) e^{i\lambda t}| dt \right) d|w|(\lambda) = \int_{\mathbb{R}} \left(\int_{\mathbb{R}} |\hat{f}(t)| dt \right) d|w|(\lambda) < \infty, \quad (2.2.14)$$

where the last inequality follows from the fact that $\hat{f} \in L^1(\mathbb{R})$ and $|w|(\cdot)$ is a finite positive measure on \mathbb{R} . Since \mathbb{R} is a σ -finite measure space with respect to the Lebesgue measure and (2.2.14) holds, by Fubini's theorem the equation (2.2.13) can be written as

$$\langle f(H_0)x, y \rangle = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \left(\int_{\mathbb{R}} e^{i\lambda t} dw(\lambda) \right) \hat{f}(t) dt.$$

By [Appendix, Theorem 4.3.6 (5)], the last expression becomes

$$\langle f(H_0)x, y \rangle = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \langle e^{iH_0 t} x, y \rangle \hat{f}(t) dt = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \langle \hat{f}(t) e^{iH_0 t} x, y \rangle dt. \quad (2.2.15)$$

By Lemma 2.2.12, for $x \in \mathcal{H}$, the function $t \mapsto \hat{f}(t) e^{iH_0 t} x$ from \mathbb{R} to \mathcal{H} is Bochner integrable and, hence, there exists a sequence of simple functions $\{s_n^{H_0, x}\}$ such that

$$\hat{f}(t) e^{iH_0 t} x = \lim_{n \rightarrow \infty} s_n^{H_0, x}(t)$$

almost everywhere and

$$\int_{\mathbb{R}} \hat{f}(t) e^{iH_0 t} x \, dt = \lim_{n \rightarrow \infty} \int_{\mathbb{R}} s_n^{H_0, x}(t) \, dt$$

in \mathcal{H} . By the continuity of an inner product, for all $y \in \mathcal{H}$, we have

$$\langle \hat{f}(t) e^{iH_0 t} x, y \rangle = \lim_{n \rightarrow \infty} \langle s_n^{H_0, x}(t), y \rangle \quad (2.2.16)$$

almost everywhere and

$$\begin{aligned} \left\langle \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{iH_0 t} x \, dt, y \right\rangle &= \frac{1}{\sqrt{2\pi}} \lim_{n \rightarrow \infty} \left\langle \int_{\mathbb{R}} s_n^{H_0, x}(t) \, dt, y \right\rangle \\ &= \frac{1}{\sqrt{2\pi}} \lim_{n \rightarrow \infty} \int_{\mathbb{R}} \langle s_n^{H_0, x}(t), y \rangle \, dt. \end{aligned} \quad (2.2.17)$$

For all $y \in \mathcal{H}$, we have

$$\begin{aligned} &\lim_{n \rightarrow \infty} \left| \int_{\mathbb{R}} \langle s_n^{H_0, x}(t), y \rangle \, dt - \int_{\mathbb{R}} \langle \hat{f}(t) e^{iH_0 t} x, y \rangle \, dt \right| \\ &= \lim_{n \rightarrow \infty} \left| \int_{\mathbb{R}} \langle s_n^{H_0, x}(t) - \hat{f}(t) e^{iH_0 t} x, y \rangle \, dt \right| \\ &\leq \lim_{n \rightarrow \infty} \int_{\mathbb{R}} \left| \langle s_n^{H_0, x}(t) - \hat{f}(t) e^{iH_0 t} x, y \rangle \right| \, dt \\ &\leq \lim_{n \rightarrow \infty} \int_{\mathbb{R}} \left\| s_n^{H_0, x}(t) - \hat{f}(t) e^{iH_0 t} x \right\| \|y\| \, dt \rightarrow 0, \end{aligned}$$

as $n \rightarrow \infty$ by the Bochner integrability of the function $t \mapsto \hat{f}(t) e^{iH_0 t} x$ (see [Appendix, Definition 4.4.4]). Therefore, we have

$$\int_{\mathbb{R}} \langle \hat{f}(t) e^{iH_0 t} x, y \rangle \, dt = \lim_{n \rightarrow \infty} \int_{\mathbb{R}} \langle s_n^{H_0, x}(t), y \rangle \, dt. \quad (2.2.18)$$

By (2.2.17) and (2.2.18), we get

$$\left\langle \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{iH_0 t} dt x, y \right\rangle = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \langle \hat{f}(t) e^{iH_0 t} x, y \rangle \, dt, \quad \text{for all } y \in \mathcal{H}.$$

Using the last equality, (2.2.15) can be written as

$$\langle f(H_0)x, y \rangle = \left\langle \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{iH_0 t} dt x, y \right\rangle, \quad \text{for all } y \in \mathcal{H},$$

and, hence

$$f(H_0)x = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{iH_0 t} x \, dt.$$

Since $x \in \mathcal{H}$ was arbitrary, we have

$$f(H_0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{iH_0 t} dt.$$

If H_0 is bounded, then the last integral converges in the uniform operator topology by Lemma 2.2.12. \square

Theorem 2.2.14. *Let $H_0 = H_0^*$ be an operator in \mathcal{H} and $V = V^* \in \mathcal{B}(\mathcal{H})$. If f is such that $f^{(j)}, \widehat{f^{(j)}} \in L^1(\mathbb{R})$, $j = 0, 1, \dots, n$, then*

$$\begin{aligned} & \left. \frac{d^n}{dt^n} \right|_{t=0} f(H_0 + tV) \\ &= n! \cdot \frac{i^n}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^{s_0} \dots \int_0^{s_{n-1}} \hat{f}(s_0) e^{i(s_0-s_1)H_0} V \dots V e^{i(s_{n-1}-s_n)H_0} V e^{is_n H_0} ds_n \dots ds_0, \end{aligned}$$

where the integral on the right is a Bochner integral and its convergence is understood in the strong operator topology. Moreover, if H_0 is bounded, then the integral can be evaluated in the uniform operator topology.

Proof. The theorem can be proved by induction on n . Here, we give the proof only for $n = 1, 2$. We first prove for $n = 1$. By Lemma 2.2.13, we have

$$\begin{aligned} f(H_0 + tV) - f(H_0) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(\lambda) e^{i\lambda(H_0+tV)} d\lambda - \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(\lambda) e^{i\lambda H_0} d\lambda \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(\lambda) (e^{i\lambda(H_0+tV)} - e^{i\lambda H_0}) d\lambda. \end{aligned} \quad (2.2.19)$$

Using Lemma 2.2.10, the equation (2.2.19) can be written as

$$\begin{aligned} f(H_0 + tV) - f(H_0) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(\lambda) \left(\int_0^\lambda e^{i(\lambda-x)(H_0+tV)} i t V e^{ixH_0} dx \right) d\lambda \\ &= \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)(H_0+tV)} t V e^{ixH_0} dx d\lambda. \end{aligned} \quad (2.2.20)$$

By the definition of first order operator derivative and using (2.2.20), we get

$$\begin{aligned} \left. \frac{d}{dt} \right|_{t=0} f(H_0 + tV) &= \lim_{t \rightarrow 0} \frac{f(H_0 + tV) - f(H_0)}{t} \\ &= \frac{i}{\sqrt{2\pi}} \lim_{t \rightarrow 0} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)(H_0+tV)} V e^{ixH_0} dx d\lambda. \end{aligned} \quad (2.2.21)$$

Using Lemma 2.2.11, we have

$$\lim_{t \rightarrow 0} \hat{f}(\lambda) e^{i(\lambda-x)(H_0+tV)} V e^{ixH_0} = \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{ixH_0}, \quad \lambda, x \in \mathbb{R},$$

where the limit is evaluated in the strong operator topology. We have

$$\left\| \hat{f}(\lambda) e^{i(\lambda-x)(H_0+tV)} V e^{ixH_0} \right\| \leq |\hat{f}(\lambda)| \|V\|.$$

Also, we have

$$\begin{aligned} & \left| \int_{\mathbb{R}} \int_0^\lambda |\hat{f}(\lambda)| \|V\| dx d\lambda \right| \\ &= \|V\| \left| \int_{\mathbb{R}} |\hat{f}(\lambda)| \left(\int_0^\lambda dx \right) d\lambda \right| \\ &\leq \|V\| \int_{\mathbb{R}} |\lambda| |\hat{f}(\lambda)| d\lambda \\ &= \|V\| \int_{\mathbb{R}} |i\lambda \hat{f}(\lambda)| d\lambda. \end{aligned}$$

Since $\widehat{f'}(\lambda) = i\lambda \hat{f}(\lambda)$ (see [Appendix, Proposition 4.5.6]) and $\widehat{f'}(\lambda) \in L^1(\mathbb{R})$, the latter estimate becomes

$$\left| \int_{\mathbb{R}} \int_0^\lambda |\hat{f}(\lambda)| \|V\| dx d\lambda \right| \leq \|V\| \int_{\mathbb{R}} |\widehat{f'}(\lambda)| d\lambda < \infty.$$

Therefore, by [Appendix, Proposition 4.4.6], the function $\hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{ixH_0}$ is Bochner integrable with respect to the Lebesgue measure $dx \times d\lambda$ and

$$\begin{aligned} & \frac{i}{\sqrt{2\pi}} \lim_{t \rightarrow 0} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)(H_0+tV)} V e^{ixH_0} dx d\lambda \\ &= \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{ixH_0} dx d\lambda. \end{aligned}$$

Using the last equality, (2.2.21) becomes

$$\left. \frac{d}{dt} \right|_{t=0} f(H_0 + tV) = \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{ixH_0} dx d\lambda. \quad (2.2.22)$$

Making the substitution $\lambda = s_0$ and $x = s_1$, the latter integral becomes

$$\left. \frac{d}{dt} \right|_{t=0} f(H_0 + tV) = \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^{s_0} \hat{f}(s_0) e^{i(s_0-s_1)H_0} V e^{is_1H_0} ds_1 ds_0$$

and, hence, the theorem is proved for $n = 1$.

Next, we prove for $n = 2$. As in the equality (2.2.22), we can show

$$\left. \frac{d}{ds} \right|_{s=t} f(H_0 + sV) = \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)(H_0+tV)} V e^{ix(H_0+tV)} dx d\lambda. \quad (2.2.23)$$

By the definition of second order operator derivative,

$$\frac{d^2}{dt^2} \Big|_{t=0} f(H_0 + tV) = \lim_{t \rightarrow 0} \frac{\frac{d}{ds} \Big|_{s=t} f(H_0 + sV) - \frac{d}{ds} \Big|_{s=0} f(H_0 + sV)}{t}.$$

Using (2.2.22) and (2.2.23), the last expression becomes

$$\begin{aligned} & \frac{d^2}{dt^2} \Big|_{t=0} f(H_0 + tV) \\ &= \lim_{t \rightarrow 0} \frac{1}{t} \left(\frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)(H_0+tV)} V e^{ix(H_0+tV)} dx d\lambda \right. \\ & \quad \left. - \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{ixH_0} dx d\lambda \right) \\ &= \lim_{t \rightarrow 0} \frac{1}{t} \left(\frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) (e^{i(\lambda-x)(H_0+tV)} - e^{i(\lambda-x)H_0}) V e^{ix(H_0+tV)} dx d\lambda \right) \\ & \quad + \lim_{t \rightarrow 0} \frac{1}{t} \left(\frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)H_0} V (e^{ix(H_0+tV)} - e^{ixH_0}) dx d\lambda \right). \end{aligned}$$

By Lemma 2.2.10, the latter expression becomes

$$\begin{aligned} & \frac{d^2}{dt^2} \Big|_{t=0} f(H_0 + tV) \\ &= \lim_{t \rightarrow 0} \frac{1}{t} \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) \left(\int_0^{\lambda-x} e^{i(\lambda-x-y)(H_0+tV)} itV e^{iyH_0} dy \right) V e^{ix(H_0+tV)} dx d\lambda \\ & \quad + \lim_{t \rightarrow 0} \frac{1}{t} \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \hat{f}(\lambda) e^{i(\lambda-x)H_0} V \left(\int_0^x e^{i(x-y)(H_0+tV)} itV e^{iyH_0} dy \right) dx d\lambda \\ &= \frac{i^2}{\sqrt{2\pi}} \lim_{t \rightarrow 0} \int_{\mathbb{R}} \int_0^\lambda \int_0^{\lambda-x} \hat{f}(\lambda) e^{i(\lambda-x-y)(H_0+tV)} V e^{iyH_0} V e^{ix(H_0+tV)} dy dx d\lambda \\ & \quad + \frac{i^2}{\sqrt{2\pi}} \lim_{t \rightarrow 0} \int_{\mathbb{R}} \int_0^\lambda \int_0^x \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{i(x-y)(H_0+tV)} V e^{iyH_0} dy dx d\lambda. \end{aligned} \quad (2.2.24)$$

Using Lemma 2.2.11, it follows that

$$\begin{aligned} & \lim_{t \rightarrow 0} \hat{f}(\lambda) e^{i(\lambda-x-y)(H_0+tV)} V e^{iyH_0} V e^{ix(H_0+tV)} \\ &= \hat{f}(\lambda) e^{i(\lambda-x-y)H_0} V e^{iyH_0} V e^{ixH_0}, \quad \lambda, x, y \in \mathbb{R}, \end{aligned}$$

where the limit is evaluated in the strong operator topology. We have

$$\left\| \hat{f}(\lambda) e^{i(\lambda-x-y)(H_0+tV)} V e^{iyH_0} V e^{ix(H_0+tV)} \right\| \leq |\hat{f}(\lambda)| \|V\|^2.$$

Also, we have

$$\left| \int_{\mathbb{R}} \int_0^\lambda \int_0^{\lambda-x} |\hat{f}(\lambda)| \|V\|^2 dy dx d\lambda \right|$$

$$\begin{aligned}
&= \|V\|^2 \left| \int_{\mathbb{R}} |\hat{f}(\lambda)| \int_0^\lambda \left(\int_0^{\lambda-x} dy \right) dx d\lambda \right| \\
&\leq \|V\|^2 \int_{\mathbb{R}} |\hat{f}(\lambda)| \int_0^\lambda |\lambda-x| dx d\lambda \\
&\leq \|V\|^2 \int_{\mathbb{R}} |(i\lambda)^2 \hat{f}(\lambda)| d\lambda.
\end{aligned}$$

Since $\widehat{f''}(\lambda) = (i\lambda)^2 \hat{f}(\lambda)$ (see [Appendix, Proposition 4.5.6]) and $\widehat{f''}(\lambda) \in L^1(\mathbb{R})$, the latter estimate becomes

$$\left| \int_{\mathbb{R}} \int_0^\lambda \int_0^{\lambda-x} |\hat{f}(\lambda)| \|V\|^2 dy dx d\lambda \right| \leq \|V\|^2 \int_{\mathbb{R}} |\widehat{f''}(\lambda)| d\lambda < \infty.$$

Therefore, by [Appendix, Proposition 4.4.6], the function

$\hat{f}(\lambda) e^{i(\lambda-x-y)H_0} V e^{iyH_0} V e^{ixH_0}$ is Bochner integrable with respect to the Lebesgue measure $dy \times dx \times d\lambda$ and

$$\begin{aligned}
&\frac{i^2}{\sqrt{2\pi}} \lim_{t \rightarrow 0} \int_{\mathbb{R}} \int_0^\lambda \int_0^{\lambda-x} \hat{f}(\lambda) e^{i(\lambda-x-y)(H_0+tV)} V e^{iyH_0} V e^{ix(H_0+tV)} dy dx d\lambda \\
&= \frac{i^2}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \int_0^{\lambda-x} \hat{f}(\lambda) e^{i(\lambda-x-y)H_0} V e^{iyH_0} V e^{ixH_0} dy dx d\lambda.
\end{aligned}$$

Similarly, we can show that

$$\begin{aligned}
&\frac{i^2}{\sqrt{2\pi}} \lim_{t \rightarrow 0} \int_{\mathbb{R}} \int_0^\lambda \int_0^x \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{i(x-y)(H_0+tV)} V e^{iyH_0} dy dx d\lambda \\
&= \frac{i^2}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \int_0^x \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{i(x-y)H_0} V e^{iyH_0} dy dx d\lambda.
\end{aligned}$$

Using the last two equalities, (2.2.24) becomes

$$\begin{aligned}
\frac{d^2}{dt^2} \Big|_{t=0} f(H_0 + tV) &= \frac{i^2}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \int_0^{\lambda-x} \hat{f}(\lambda) e^{i(\lambda-x-y)H_0} V e^{iyH_0} V e^{ixH_0} dy dx d\lambda \\
&\quad + \frac{i^2}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^\lambda \int_0^x \hat{f}(\lambda) e^{i(\lambda-x)H_0} V e^{i(x-y)H_0} V e^{iyH_0} dy dx d\lambda.
\end{aligned} \tag{2.2.25}$$

Making the substitution $\lambda = s_0$, $x = s_2$, and $y = s_1 - s_2$ in the first integral and the substitution $\lambda = s_0$, $x = s_1$, and $y = s_2$ in the second integral of (2.2.25), we obtain the representation

$$\begin{aligned}
&\frac{d^2}{dt^2} \Big|_{t=0} f(H_0 + tV) \\
&= 2! \cdot \frac{i^2}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^{s_0} \int_0^{s_1} \hat{f}(s_0) e^{i(s_0-s_1)H_0} V e^{i(s_1-s_2)H_0} V e^{is_2H_0} ds_2 ds_1 ds_0
\end{aligned}$$

and, hence, the theorem is proved for $n = 2$.

We now assume that H_0 is bounded. Then, by Lemma 2.2.13

$$f(H_0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) e^{iH_0 t} dt,$$

where the convergence of the integral is evaluated in the uniform operator topology. Similarly, the integral and limit in Lemma 2.2.10 and Lemma 2.2.11 can be evaluated in the uniform operator topology. Using all these results and proceeding as above, we see the integral in this lemma converges in the uniform operator topology. \square

Chapter 3

Trace formulas in the case of Hilbert-Schmidt resolvents

Let the resolvent of H_0 belong to \mathcal{S}^2 , that is, $|(iI + H_0)^{-1}| = (I + H_0^2)^{-1/2} \in \mathcal{S}^2$; $V = V^* \in \mathcal{B}(\mathcal{H})$; and $f \in C_c^n((a, b))$, where $C_c^n((a, b))$ is the space of n times continuously differentiable functions on \mathbb{R} that are compactly supported in $(a, b) \subset \mathbb{R}$. We show that there exists a unique locally finite real-valued measure $\mu_n = \mu_{n, H_0, V}$, $n \geq 3$, such that the following trace formula holds (see Theorem 3.1.7):

$$\mathrm{Tr} \left(f(H_0 + V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{R}} f^{(n)}(t) d\mu_n(t),$$

for $f \in C_c^n((a, b))$. In the case of commuting H_0 and V , we show that there exists a locally integrable function $\eta_n = \eta_{n, H_0, V}$, $n \geq 3$, such that the following trace formula holds (see Theorem 3.2.1):

$$\mathrm{Tr} \left(f(H_0 + V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{R}} f^{(n)}(t) \eta_n(t) dt,$$

for $f \in C_c^n((a, b))$.

Following delicate methods of noncommutative analysis developed in [18], we first show that each summand in $f(H_0 + V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV)$ is a trace class operator (see Lemmas 3.1.1 and 3.1.5) and prove the estimate

$$\left| \mathrm{Tr} \left(f(H_0 + V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) \right| \leq C_{n, a, b, H_0, V} \cdot \|f^{(n)}\|_{\infty},$$

where $C_{n, a, b, H_0, V}$ is a constant depending on a , b , H_0 and V . Then, we use the Riesz representation theorem for a functional in $(C_c(\mathbb{R}))^*$ to find a unique locally finite

real-valued measure μ_n that satisfies the result in Theorem 3.1.7. To prove Theorem 3.2.1, we simply prove the absolute continuity of the measure μ_n obtained in Theorem 3.1.7 using integration by parts.

3.1 Non-commutative perturbations

In this section, we assume that the initial operator H_0 and its bounded perturbation V do not commute, that is, $H_0V \neq VH_0$.

3.1.1 Trace Formulas

The main result is in Theorem 3.1.7. We have several auxiliary lemmas before the main result.

Lemma 3.1.1. (See [18, Lemma 2.5]) *Let $H_0 = H_0^*$ satisfy $(I + H_0^2)^{-1/2} \in \mathcal{S}^2$ and let $V = V^* \in \mathcal{B}(\mathcal{H})$. Let f be a continuous compactly supported function on \mathbb{R} . Then, $f(H_0 + V) \in \mathcal{S}^1$ and*

$$\|f(H_0 + V)\|_1 \leq \|f\|_\infty \cdot \left(1 + \max_{s \in \text{supp} f} |s|^2\right) \cdot (1 + \|V\| + \|V\|^2) \cdot \|(I + H_0^2)^{-1/2}\|_2^2.$$

In particular, $f(H_0) \in \mathcal{S}^1$ and

$$\|f(H_0)\|_1 \leq \|f\|_\infty \cdot \left(1 + \max_{s \in \text{supp} f} |s|^2\right) \cdot \|(I + H_0^2)^{-1/2}\|_2^2.$$

Lemma 3.1.2. (See [3, Lemma 2.1]) *If f is such that $f^{(j)}, \widehat{f^{(j)}} \in L^1(\mathbb{R})$, $j = 0, 1, \dots, n$, then*

$$\begin{aligned} & f^{[n]}[\lambda_0, \dots, \lambda_n] \\ &= \frac{i^n}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^{s_0} \dots \int_0^{s_{n-1}} \widehat{f}(s_0) e^{i(s_0-s_1)\lambda_0} \dots e^{i(s_{n-1}-s_n)\lambda_{n-1}} e^{is_n\lambda_n} ds_n \dots ds_0, \end{aligned}$$

where $f^{[n]}[\lambda_0, \dots, \lambda_n]$ is a divided difference of order n given by Definition 2.1.1.

Lemma 3.1.3. (See [3, Lemma 4.5]) *Let $H_0 = H_0^*, \dots, H_n = H_n^*$ be defined in \mathcal{H} and let $V_1, \dots, V_n \in \mathcal{B}(\mathcal{H})$. If f is such that $f^{(j)}, \widehat{f^{(j)}} \in L^1(\mathbb{R})$, $j = 0, 1, \dots, n$, then the Bochner integral*

$$T_{f^{[n]}}^{H_0, \dots, H_n}(V_1, \dots, V_n)y \tag{3.1.1}$$

$$:= \frac{i^n}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^{s_0} \dots \int_0^{s_{n-1}} \widehat{f}(s_0) e^{i(s_0-s_1)H_0} V_1 \dots V_{n-1} e^{i(s_{n-1}-s_n)H_{n-1}} V_n e^{is_n H_n} y ds_n \dots ds_0 \tag{3.1.2}$$

exists for every $y \in \mathcal{H}$ and thus defines a bounded linear operator on \mathcal{H} with the norm bound

$$\left\| T_{f^{[n]}}^{H_0, \dots, H_n}(V_1, \dots, V_n) \right\| \leq \frac{1}{n!} \cdot \left\| \widehat{f^{(n)}} \right\|_1 \cdot \|V_1\| \cdot \dots \cdot \|V_n\|.$$

Remark 3.1.4. $T_{f^{[n]}}^{H_0, \dots, H_n}(V_1, \dots, V_n)$ in the above lemma is a bounded multilinear mapping from $\mathcal{B}(\mathcal{H}) \times \dots \times \mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\mathcal{H})$. It follows immediately from Theorem 2.2.14 and (3.1.2) that for $V = V^* \in \mathcal{B}(\mathcal{H})$ and f is such that $f^{(j)}, \widehat{f^{(j)}} \in L^1(\mathbb{R}), j = 0, 1, \dots, n$,

$$\frac{1}{n!} \cdot \frac{d^n}{dt^n} \Big|_{t=0} f(H_0 + tV) = T_{f^{[n]}}^{H_0, \dots, H_0} \underbrace{(V, \dots, V)}_{n \text{ times}}.$$

Lemma 3.1.5. (See [18, Lemma 3.6]) Let $H_0 = H_0^*$ satisfy $(I + H_0^2)^{-1/2} \in \mathcal{S}^2$ and let $V = V^* \in \mathcal{B}(\mathcal{H})$. Denote $u(t) = (1 + t^2)^{1/2}$. Then, for every $n \in \mathbb{N}$ and $f \in C_c^{n+1}(\mathbb{R})$, $\frac{1}{n!} \cdot \frac{d^n}{dt^n} \Big|_{t=0} f(H_0 + tV) \in \mathcal{S}^1$ and

$$\left\| \frac{1}{n!} \cdot \frac{d^n}{dt^n} \Big|_{t=0} f(H_0 + tV) \right\|_1 \leq C_{f,n} \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \cdot \|V\|^n,$$

where

$$C_{f,1} \leq \sqrt{2} \left(\|(fu^2)'\|_2 + \|(fu^2)''\|_2 \right) + 2\|fu^2\|_\infty \quad (3.1.3)$$

and for $n \geq 2$,

$$\begin{aligned} C_{f,n} &\leq \frac{\sqrt{2}}{n!} \left(\|(fu^2)^{(n)}\|_2 + \|(fu^2)^{(n+1)}\|_2 \right) \\ &\quad + \frac{n(n+3)}{2} \cdot \max_{1 \leq k \leq n} \left\{ \|f\|_\infty, \|fu\|_\infty, \frac{\sqrt{2}}{k!} \left(\|f^{(k)}\|_2 + \|f^{(k+1)}\|_2 \right), \right. \\ &\quad \left. \frac{\sqrt{2}}{k!} \left(\|(fu)^{(k)}\|_2 + \|(fu)^{(k+1)}\|_2 \right) \right\} \\ &\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left(\|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2. \end{aligned} \quad (3.1.4)$$

Lemma 3.1.6. Let $f \in C_c^{n+1}((a, b))$, $n \in \mathbb{N}$, and $u(t) = (1 + t^2)^{1/2}$. If $C_{f,n}$ satisfy (3.1.3) for $n = 1$ and (3.1.4) for $n \geq 2$, then

$$C_{f,n} \leq \|f^{(n+1)}\|_\infty \cdot C_{a,b,n}, \quad n \in \mathbb{N}, \quad (3.1.5)$$

where

$$C_{a,b,1} = 24 \cdot \max \left\{ 1, (b-a)^2 \right\} \cdot \max \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])} \right\} \quad (3.1.6)$$

and for $n \geq 2$,

$$\begin{aligned}
C_{a,b,n} &= \left[\frac{4(b-a)^{1/2}}{n!} + \frac{n(n+3)}{2} \cdot \max \left\{ 1, 4(b-a)^{1/2} \right\} \right. \\
&\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left(\|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2 \left. \right] \cdot 2^n \cdot \max \left\{ 1, (b-a)^{n+1} \right\} \\
&\quad \times \max_{0 \leq k \leq n+1} \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \|u^{(k)}\|_{L^\infty([a,b])} \right\}. \quad (3.1.7)
\end{aligned}$$

Proof. We prove the case $n \geq 2$. The case $n = 1$ is similar to that of $n \geq 2$ and, hence, omitted. Here, we denote $\|\cdot\|_2 = \|\cdot\|_{L^2([a,b])}$ and $\|\cdot\|_\infty = \|\cdot\|_{L^\infty([a,b])}$. For $f \in C_c^{n+1}((a,b))$,

$$\|f^{(j)}\|_2 \leq \|f^{(j)}\|_\infty \cdot (b-a)^{1/2}, \quad 0 \leq j \leq n+1. \quad (3.1.8)$$

Using (3.1.8), we obtain that

$$\begin{aligned}
&C_{f,n} \\
&\leq \frac{\sqrt{2}}{n!} \left(\|(fu^2)^{(n)}\|_\infty (b-a)^{1/2} + \|(fu^2)^{(n+1)}\|_\infty (b-a)^{1/2} \right) \\
&\quad + \frac{n(n+3)}{2} \cdot \max_{1 \leq k \leq n} \left\{ \|f\|_\infty, \|fu\|_\infty, \frac{\sqrt{2}}{k!} \left(\|f^{(k)}\|_\infty (b-a)^{1/2} + \|f^{(k+1)}\|_\infty (b-a)^{1/2} \right), \right. \\
&\quad \left. \frac{\sqrt{2}}{k!} \left(\|(fu)^{(k)}\|_\infty (b-a)^{1/2} + \|(fu)^{(k+1)}\|_\infty (b-a)^{1/2} \right) \right\} \\
&\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left(\|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2. \quad (3.1.9)
\end{aligned}$$

Since

$$\begin{aligned}
\|(fg)^{(k)}\|_\infty &= \left\| \sum_{j=0}^k \binom{k}{j} f^{(j)} g^{(k-j)} \right\|_\infty \leq \sum_{j=0}^k \binom{k}{j} \|f^{(j)}\|_\infty \|g^{(k-j)}\|_\infty \\
&\leq 2^k \cdot \max_{0 \leq j \leq k} \|f^{(j)}\|_\infty \cdot \max_{0 \leq l \leq k} \|g^{(l)}\|_\infty,
\end{aligned}$$

for $0 \leq i \leq n+1$, we have

$$\begin{aligned}
\|(fu^2)^{(i)}\|_\infty &\leq 2^i \cdot \max_{0 \leq j \leq i} \|f^{(j)}\|_\infty \cdot \max_{0 \leq l \leq i} \|(u^2)^{(l)}\|_{L^\infty([a,b])} \\
&\leq 2^{n+1} \cdot \max \left\{ \|f\|_\infty, \|f'\|_\infty, \dots, \|f^{(n+1)}\|_\infty \right\} \\
&\quad \times \max \left\{ \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \dots, \|(u^2)^{(n+1)}\|_{L^\infty([a,b])} \right\}. \quad (3.1.10)
\end{aligned}$$

Since, for $f \in C_c^{n+1}((a,b))$,

$$\|f^{(j)}\|_\infty \leq \|f^{(n+1)}\|_\infty \cdot (b-a)^{n+1-j}, \quad 0 \leq j \leq n+1,$$

(3.1.10) is bounded by

$$\begin{aligned} \|(fu^2)^{(i)}\|_\infty &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max \left\{ (b-a)^{n+1}, (b-a)^n, \dots, 1 \right\} \\ &\quad \times \max \left\{ \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \dots, \|(u^2)^{(n+1)}\|_{L^\infty([a,b])} \right\}, \end{aligned} \quad (3.1.11)$$

for $0 \leq i \leq n+1$. Since $\max_{1 \leq i \leq n+1} \{1, (b-a)^i\} \leq \max\{1, (b-a)^{n+1}\}$, $(u^2)'' \equiv 2$, and $(u^2)^{(n+1)} = 0$, for $n \geq 2$, (3.1.11) is bounded by

$$\begin{aligned} &\|(fu^2)^{(i)}\|_\infty \\ &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max \left\{ 1, (b-a)^{n+1} \right\} \cdot \max \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])} \right\} \\ &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max \left\{ 1, (b-a)^{n+1} \right\} \\ &\quad \times \max_{0 \leq k \leq n+1} \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \|u^{(k)}\|_{L^\infty([a,b])} \right\}, \quad 0 \leq i \leq n+1. \end{aligned} \quad (3.1.12)$$

Similarly, for $0 \leq i \leq n+1$, we have

$$\begin{aligned} &\|f^{(i)}\|_\infty \\ &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max \left\{ 1, (b-a)^{n+1} \right\} \\ &\quad \times \max_{0 \leq k \leq n+1} \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \|u^{(k)}\|_{L^\infty([a,b])} \right\}. \end{aligned} \quad (3.1.13)$$

and

$$\begin{aligned} &\|(fu)^{(i)}\|_\infty \\ &\leq 2^{n+1} \cdot \|f^{(n+1)}\|_\infty \cdot \max \left\{ 1, (b-a)^{n+1} \right\} \\ &\quad \times \max_{0 \leq k \leq n+1} \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \|u^{(k)}\|_{L^\infty([a,b])} \right\}. \end{aligned} \quad (3.1.14)$$

Using (3.1.12)–(3.1.14), we obtain that

$$\begin{aligned} C_{f,n} &\leq \|f^{(n+1)}\|_\infty \cdot \left[\frac{2^{3/2}(b-a)^{1/2}}{n!} + \frac{n(n+3)}{2} \cdot \max \left\{ 1, 2^{3/2}(b-a)^{1/2} \right\} \right. \\ &\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left(\|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2 \left. \right] \cdot 2^n \cdot \max \left\{ 1, (b-a)^{n+1} \right\} \\ &\quad \times \max_{0 \leq k \leq n+1} \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \|u^{(k)}\|_{L^\infty([a,b])} \right\} \\ &\leq \|f^{(n+1)}\|_\infty \cdot \left[\frac{4(b-a)^{1/2}}{n!} + \frac{n(n+3)}{2} \cdot \max \left\{ 1, 4(b-a)^{1/2} \right\} \right. \\ &\quad \times \text{const} \cdot \max_{2 \leq j \leq n} \left(\|u^{(j)}\|_2 + \|u^{(j+1)}\|_2 \right)^2 \left. \right] \cdot 2^n \cdot \max \left\{ 1, (b-a)^{n+1} \right\} \\ &\quad \times \max_{0 \leq k \leq n+1} \left\{ 2, \|u^2\|_{L^\infty([a,b])}, \|(u^2)'\|_{L^\infty([a,b])}, \|u^{(k)}\|_{L^\infty([a,b])} \right\} \\ &= \|f^{(n+1)}\|_\infty \cdot C_{a,b,n}, \quad n \geq 2, \end{aligned}$$

where $C_{a,b,n}$ is given by (3.1.7). \square

Theorem 3.1.7. *Let $H_0 = H_0^*$ satisfy $(I + H_0^2)^{-1/2} \in \mathcal{S}^2$ and let $V = V^* \in \mathcal{B}(\mathcal{H})$. Then, there is a unique locally finite real-valued measure $\mu_n = \mu_{n,H_0,V}$, $n \geq 3$, with total variation on the segment $[a, b]$*

$$\int_{[a,b]} d|\mu_n| \leq 2 \cdot C_{a,b} \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \cdot \sum_{k=0}^{n-1} \|V\|^k, \quad (3.1.15)$$

where

$$C_{a,b} = \max_{1 \leq k \leq n-1} \left\{ (b-a)^n \cdot (1 + a^2 + b^2), C_{a,b,k} \cdot (b-a)^{n-1-k} \right\}, \quad n \geq 3, \quad (3.1.16)$$

$C_{a,b,k}$ is given by (3.1.6) for $k = 1$ and (3.1.7) for $k \geq 2$, such that

$$\mathrm{Tr} \left(f(H_0 + V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{R}} f^{(n)}(\lambda) d\mu_n(\lambda),$$

for $f \in C_c^n((a, b))$, $a, b \in \mathbb{R}$.

Proof. Let $n \geq 3$ and let

$$R_{n,H_0,V}(f) := f(H_0 + V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV). \quad (3.1.17)$$

By Lemmas 3.1.1 and 3.1.5, each summand on the right hand side of (3.1.17) is a trace class operator. Therefore, taking trace on both sides of (3.1.17) and using the linearity of the trace functional, we get

$$\mathrm{Tr}(R_{n,H_0,V}(f)) = \mathrm{Tr}(f(H_0 + V)) - \mathrm{Tr}(f(H_0)) - \sum_{k=1}^{n-1} \mathrm{Tr} \left(\frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right).$$

Using the triangle inequality, we get from the last expression

$$\begin{aligned} & \left| \mathrm{Tr}(R_{n,H_0,V}(f)) \right| \\ & \leq \left| \mathrm{Tr}(f(H_0 + V)) \right| + \left| \mathrm{Tr}(f(H_0)) \right| + \sum_{k=1}^{n-1} \left| \mathrm{Tr} \left(\frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) \right|. \end{aligned}$$

Since for $A \in \mathcal{S}^1$, $|\mathrm{Tr}(A)| \leq \|A\|_1$, the latter expression is bounded by

$$\left| \mathrm{Tr}(R_{n,H_0,V}(f)) \right| \leq \|f(H_0 + V)\|_1 + \|f(H_0)\|_1 + \sum_{k=1}^{n-1} \left\| \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right\|_1. \quad (3.1.18)$$

Again by Lemmas 3.1.1 and 3.1.5, (3.1.18) is bounded by

$$\begin{aligned} & \left| \text{Tr}(R_{n,H_0,V}(f)) \right| \\ & \leq \left(\|f\|_\infty \cdot \left(1 + \max_{s \in \text{supp}f \subset (a,b)} |s|^2 \right) \cdot (2 + \|V\| + \|V\|^2) + \sum_{k=1}^{n-1} C_{f,k} \cdot \|V\|^k \right) \\ & \quad \times \|(I + H_0^2)^{-1/2}\|_2^2, \end{aligned} \quad (3.1.19)$$

where $C_{f,k}$ satisfies (3.1.3) for $k = 1$ and (3.1.4) for $k \geq 2$. By Lemma 3.1.6 and the fact that $(1 + \max_{s \in \text{supp}f \subset (a,b)} |s|^2) \leq (1 + a^2 + b^2)$ applied in (3.1.19),

$$\begin{aligned} & \left| \text{Tr}(R_{n,H_0,V}(f)) \right| \\ & \leq \left(\|f\|_\infty \cdot (1 + a^2 + b^2) \cdot (2 + \|V\| + \|V\|^2) + \sum_{k=1}^{n-1} \|f^{(k+1)}\|_\infty \cdot C_{a,b,k} \cdot \|V\|^k \right) \\ & \quad \times \|(I + H_0^2)^{-1/2}\|_2^2, \end{aligned}$$

where $C_{a,b,k}$ is given by (3.1.6) for $k = 1$ and (3.1.7) for $k \geq 2$. For $f \in C_c^n((a, b))$,

$$\|f^{(j)}\|_\infty \leq \|f^{(n)}\|_\infty \cdot (b - a)^{n-j}, \quad 0 \leq j \leq n,$$

and, hence,

$$\begin{aligned} & \left| \text{Tr}(R_{n,H_0,V}(f)) \right| \\ & \leq \|f^{(n)}\|_\infty \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \\ & \quad \times \left((b - a)^n \cdot (1 + a^2 + b^2) \cdot (2 + \|V\| + \|V\|^2) + \sum_{k=1}^{n-1} C_{a,b,k} \cdot (b - a)^{n-1-k} \cdot \|V\|^k \right). \end{aligned} \quad (3.1.20)$$

If $C_{a,b}$ is given by (3.1.16), then(3.1.20) is bounded by

$$\begin{aligned} \left| \text{Tr}(R_{n,H_0,V}(f)) \right| & \leq C_{a,b} \cdot \|f^{(n)}\|_\infty \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \cdot \left(2 + \|V\| + \|V\|^2 + \sum_{k=1}^{n-1} \|V\|^k \right) \\ & \leq 2 \cdot C_{a,b} \cdot \|f^{(n)}\|_\infty \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \cdot \sum_{k=0}^{n-1} \|V\|^k. \end{aligned}$$

Hence, by the Riesz representation theorem for a functional in $(C_c(\mathbb{R}))^*$, there is a unique locally finite real-valued measure $\mu_n = \mu_{n,H_0,V}$, $n \geq 3$, with total variation on the segment $[a, b]$ satisfying (3.1.15) such that

$$\text{Tr}(R_{n,H_0,V}(f)) = \int_{\mathbb{R}} f^{(n)}(\lambda) d\mu_n(\lambda).$$

□

3.1.2 Example of a Self-adjoint operator with Hilbert-Schmidt resolvent

In this section, we will make a specific choice of a Hilbert space \mathcal{H} and a self-adjoint operator H_0 with Hilbert-Schmidt resolvent to which Theorem 3.1.7 applies. More precisely, we take $\mathcal{H} = L^2([0, \pi])$ and H_0 a negative Laplacian with Dirichlet boundary conditions. We show that H_0 is self-adjoint (see Lemma 3.1.15) with Hilbert-Schmidt resolvent (see Lemma 3.1.17) so that if $V = V^*$ is any bounded perturbation, then the result in Theorem 3.1.7 holds.

Let $\mathcal{H} = L^2([0, \pi])$ and denote

$$\mathcal{D} = \{f \in \mathcal{H} : f' \text{ exists, } f' \text{ is absolutely continuous, } f'' \in \mathcal{H}, \text{ and } f(0) = f(\pi) = 0\}. \quad (3.1.21)$$

Let $H_0 : \mathcal{D} \mapsto \mathcal{H}$ be defined by

$$H_0 u = -u''. \quad (3.1.22)$$

The operator H_0 given by the equation (3.1.22) is called a Sturm-Liouville operator. We will see that eigenvalues of H_0 are real numbers and the resolvent operator $(H_0 - \lambda I)^{-1}$ of H_0 , where $\lambda \in \mathbb{R}$ is not an eigenvalue of H_0 is a compact self-adjoint operator. In order to compute the resolvent, we solve the inhomogeneous equation

$$(H_0 - \lambda I)u = f, \quad u(0) = 0 = u(\pi).$$

We will show that $(H_0 - \lambda I)^{-1}$ is an integral operator with square integrable kernel called Green's function of the Sturm-Liouville problem. Then, it follows that the operator $(H_0 - \lambda I)^{-1}$, $\lambda \in \mathbb{R}$ is not an eigenvalue of H_0 , is a compact self-adjoint operator. Finally, we show that the resolvent operator $(H_0 - \lambda I)^{-1}$ belongs to \mathcal{S}^2 .

Definition 3.1.8. (See, e.g., [1, Section 2.4]) *Green's function for the Sturm-Liouville operator given by the equation (3.1.22) is a function*

$$g : [0, \pi] \times [0, \pi] \mapsto \mathbb{R}$$

with the following properties:

1. g is symmetric, in the sense that

$$g(x, y) = g(y, x) \quad \text{for all } x, y \in [0, \pi],$$

and g satisfies the boundary conditions in each variable x and y .

2. g is a continuous function on the square $[0, \pi] \times [0, \pi]$ and of class C^2 on $[0, \pi] \times [0, \pi] \setminus \{(x, y) : x = y\}$, where it satisfies the differential equation

$$g_{xx}(x, y) = 0.$$

3. The derivative g_x has a jump discontinuity at $x = y$ given by

$$g_x(y+, y) - g_x(y-, y) = \lim_{c \rightarrow y+} g_x(c, y) - \lim_{c \rightarrow y-} g_x(c, y) = -1.$$

Lemma 3.1.9. Let $H_0 : \mathcal{D} \mapsto \mathcal{H}$, where \mathcal{D} is defined by the equation (3.1.21) be given by

$$H_0 u = -u''$$

and assume that

$$H_0 u = 0 \implies u = 0.$$

Then, the Green function g for H_0 satisfying the Definition 3.1.8 is given by

$$g(x, y) = \begin{cases} \frac{x(\pi - y)}{\pi}, & 0 \leq x \leq y \leq \pi \\ \frac{y(\pi - x)}{\pi}, & 0 \leq y \leq x \leq \pi. \end{cases} \quad (3.1.23)$$

Proof. Let us choose non-zero solutions

$$u_1(x) = x$$

and

$$u_2(x) = \pi - x$$

of $H_0 u = 0$ such that u_1 satisfies the boundary condition at $x = 0$,

$$u_1(0) = 0,$$

and u_2 satisfies the boundary condition at $x = \pi$,

$$u_2(\pi) = 0.$$

Since the Wronskian W of u_1 and u_2 satisfies

$$\begin{aligned} W(y) &= \begin{vmatrix} u_1(y) & u_2(y) \\ u_1'(y) & u_2'(y) \end{vmatrix} \\ &= u_1(y)u_2'(y) - u_2(y)u_1'(y) \\ &= y(-1) - (\pi - y)(1) \\ &= -\pi \neq 0, \text{ for all } y \in [0, \pi], \end{aligned}$$

u_1 and u_2 are linearly independent.

Now define

$$\begin{aligned} g(x, y) &= \begin{cases} C(y)u_1(x)u_2(y), & 0 \leq x \leq y \leq \pi \\ C(y)u_1(y)u_2(x), & 0 \leq y \leq x \leq \pi \end{cases} \\ &= \begin{cases} C(y)x(\pi - y), & 0 \leq x \leq y \leq \pi \\ C(y)y(\pi - x), & 0 \leq y \leq x \leq \pi, \end{cases} \end{aligned} \quad (3.1.24)$$

where

$$C(y) = -\frac{1}{W(y)} = \frac{1}{\pi}.$$

Substituting the value of $C(y)$ in the equation (3.1.24), we get the equation (3.1.23).

Now it remains to show that all the properties of $g(x, y)$ listed in the Definition 3.1.8 are satisfied. Clearly, $g(x, y) = g(y, x)$ and hence g is symmetric. By the equation (3.1.23), it follows that

$$g(0, y) = 0 = g(\pi, y) \quad \text{and} \quad g(x, 0) = 0 = g(x, \pi),$$

which shows that g satisfies the boundary conditions in each variable x and y . Thus, the property 1 of Definition 3.1.8 is satisfied. The function g is obviously continuous on $[0, \pi] \times [0, \pi]$. Differentiating the equation (3.1.23) with respect to x , we get

$$g_x(x, y) = \begin{cases} \frac{(\pi - y)}{\pi}, & 0 \leq x < y \leq \pi \\ \frac{-y}{\pi}, & 0 \leq y < x \leq \pi. \end{cases}$$

Therefore,

$$g_{xx}(x, y) = 0 \quad \text{for } x \neq y.$$

Thus, the property 2 of Definition 3.1.8 is satisfied. Finally,

$$\begin{aligned} g_x(y+, y) - g_x(y-, y) &= \lim_{c \rightarrow y+} g_x(c, y) - \lim_{c \rightarrow y-} g_x(c, y) \\ &= \lim_{c \rightarrow y+} -\frac{y}{\pi} - \lim_{c \rightarrow y-} \frac{\pi - y}{\pi} \\ &= -1, \end{aligned}$$

which proves that property 3 of Definition 3.1.8 is also satisfied. \square

Theorem 3.1.10. (See, e.g., [6, Chapter II, Proposition 4.7]) Let (X, Ω, μ) be a finite measure space and let $k \in L^2(X \times X, \Omega \times \Omega, \mu \times \mu)$. Then, the integral operator $K : L^2(X, \Omega, \mu) \mapsto L^2(X, \Omega, \mu)$ defined by

$$(Kf)(x) = \int_X k(x, y)f(y)d\mu(y)$$

is a compact operator and $\|K\| \leq \|k\|_{\mathcal{L}^2}$.

The theorem below is a known result. We give here a simple and rigorous proof for it.

Theorem 3.1.11. (See, e.g., [6, [Chapter II, Theorem 6.9]]) Let $H_0 : \mathcal{D} \mapsto \mathcal{H}$, where \mathcal{D} is defined by the equation (3.1.21), be given by

$$H_0u = -u''$$

and assume that

$$H_0u = 0 \implies u = 0.$$

Let g be the Green function for H_0 given by the equation (3.1.23). Let $G : \mathcal{H} \mapsto \mathcal{H}$ be the integral operator defined by

$$(Gf)(x) = \int_0^\pi g(x, y)f(y)dy. \quad (3.1.25)$$

Then, G is a compact self-adjoint operator on \mathcal{H} , $Gf \in \mathcal{D}$ for all $f \in \mathcal{H}$, $H_0Gf = f$ for all $f \in \mathcal{H}$, and $GH_0h = h$ for all $h \in \mathcal{D}$.

Proof. Since $g(x, y)$ is continuous on $[0, \pi] \times [0, \pi]$ and $[0, \pi] \times [0, \pi]$ is compact, there exists $M > 0$ such that $|g(x, y)| \leq M$ for all $x, y \in [0, \pi] \times [0, \pi]$. Since

$$\int_{[0, \pi] \times [0, \pi]} |g(x, y)|^2 d(x \times y) \leq M^2 \pi^2 < \infty,$$

G is compact according to Theorem 3.1.10. We now show that G is self-adjoint. For $f, h \in \mathcal{H}$,

$$\begin{aligned} \langle Gf, h \rangle &= \int_0^\pi (Gf)(x)\bar{h}(x)dx \\ &= \int_0^\pi \int_0^\pi g(x, y)f(y)\bar{h}(x)dy dx. \end{aligned}$$

Since g is real valued and symmetric, the last expression becomes

$$\langle Gf, h \rangle = \int_0^\pi \int_0^\pi \bar{g}(y, x) \bar{h}(x) f(y) dy dx \quad (3.1.26)$$

By the Hölder inequality, we get

$$\begin{aligned} \int_0^\pi |f(y)| dy &\leq \left(\int_0^\pi 1 dy \right)^{1/2} \left(\int_0^\pi |f(y)|^2 dy \right)^{1/2} \\ &= \sqrt{\pi} \left(\int_0^\pi |f(y)|^2 dy \right)^{1/2} < \infty. \end{aligned}$$

Similarly, we can show

$$\int_0^\pi |\bar{h}(x)| dx < \infty.$$

Also, we have $|\bar{g}(y, x)| = |g(x, y)| \leq M$ for all $x, y \in [0, \pi] \times [0, \pi]$. Therefore, we have

$$\int_0^\pi \left(\int_0^\pi |\bar{g}(y, x) \bar{h}(x) f(y)| dy \right) dx < \infty. \quad (3.1.27)$$

Since $[0, \pi]$ is a finite measure space with respect to the Lebesgue measure and the equation (3.1.27) holds, by Fubini's theorem the equation (3.1.26) can be written as

$$\begin{aligned} \langle Gf, h \rangle &= \int_0^\pi f(y) \int_0^\pi \bar{g}(y, x) \bar{h}(x) dx dy \\ &= \int_0^\pi f(y) \overline{Gh}(y) dy \\ &= \langle f, Gh \rangle, \end{aligned}$$

which proves that G is self-adjoint.

Let us fix some $f \in \mathcal{H}$ and let $h = Gf$. We wish to show that $h \in \mathcal{D}$. We have

$$\begin{aligned} h(x) &= \int_0^\pi g(x, y) f(y) dy \\ &= \int_0^x g(x, y) f(y) dy + \int_x^\pi g(x, y) f(y) dy \\ &= \int_0^x \frac{y(\pi - x)}{\pi} f(y) dy + \int_x^\pi \frac{x(\pi - y)}{\pi} f(y) dy \\ &= \frac{\pi - x}{\pi} \int_0^x y f(y) dy + \frac{x}{\pi} \int_x^\pi (\pi - y) f(y) dy. \end{aligned}$$

By the Hölder inequality, we get

$$\int_0^\pi |y f(y)| dy \leq \left(\int_0^\pi |y|^2 dy \right)^{1/2} \left(\int_0^\pi |f(y)|^2 dy \right)^{1/2} < \infty,$$

which implies that $yf(y) \in \mathcal{L}^1([0, \pi])$. Similarly, we can show that $(\pi - y)f(y) \in L^1([0, \pi])$. Therefore,

$$h_1(x) := \int_0^x yf(y)dy$$

and

$$h_2(x) := \int_x^\pi (\pi - y)f(y)dy$$

are absolutely continuous, and

$$h_1'(x) = xf(x) \text{ for almost every } x \in [0, \pi],$$

and

$$h_2'(x) = -(\pi - x)f(x) \text{ for almost every } x \in [0, \pi].$$

Therefore, we have

$$\begin{aligned} h'(x) &= \frac{\pi - x}{\pi} xf(x) - \frac{1}{\pi} h_1(x) - \frac{x}{\pi}(\pi - x)f(x) + \frac{1}{\pi} h_2(x) \text{ for almost every } x \in [0, \pi] \\ &= \frac{1}{\pi}(h_2(x) - h_1(x)) \text{ for all } x \in [0, \pi], \end{aligned} \quad (3.1.28)$$

since h_1 and h_2 are absolutely continuous on $[0, \pi]$. Therefore, h' is also absolutely continuous on $[0, \pi]$. Differentiating the equation (3.1.28), we get

$$\begin{aligned} h''(x) &= \frac{1}{\pi}(h_2'(x) - h_1'(x)) \\ &= \frac{1}{\pi}(-(\pi - x)f(x) - xf(x)) \\ &= -f(x) \text{ for almost every } x \in [0, \pi]. \end{aligned} \quad (3.1.29)$$

Since $f \in \mathcal{H}$, $h'' \in \mathcal{H}$. Also, $h(0) = 0 = h(\pi)$. Hence, $h \in \mathcal{D}$.

To show $H_0Gf = f$ for all $f \in \mathcal{H}$, let $h = Gf$. Then, $H_0h = -h'' = f$ by the equation (3.1.29).

To show $GH_0u = u$ for all $u \in \mathcal{D}$, let $u \in \mathcal{D}$. Then, $H_0u \in \mathcal{H}$. Since $H_0Gf = f$ for all $f \in \mathcal{H}$, $H_0GH_0u = H_0u$, which implies that $H_0(GH_0u - u) = 0$. Since $\ker H_0 = \{0\}$, it follows that $GH_0u = u$ for all $u \in \mathcal{D}$. \square

Lemma 3.1.12. Let $\lambda \in \mathbb{R} \setminus \{n^2\}_{n=0}^{\infty}$. Let $L = (H_0 - \lambda I) : \mathcal{D} \mapsto \mathcal{H}$, where \mathcal{D} is defined by the equation (3.1.21), be given by

$$Lu = -u'' - \lambda u$$

and assume that

$$Lu = 0 \implies u = 0.$$

Then, the Green function g for L satisfying Definition 3.1.8 is given by

$$g(x, y) = \begin{cases} \frac{\sin \sqrt{\lambda} x \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} y)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi}, & 0 \leq x \leq y \leq \pi \\ \frac{\sin \sqrt{\lambda} y \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi}, & 0 \leq y \leq x \leq \pi. \end{cases} \quad (3.1.30)$$

Proof. Let us choose non-zero solutions

$$u_1(x) = \sin \sqrt{\lambda} x$$

and

$$u_2(x) = \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x)$$

of $Lu = 0$ such that u_1 satisfies the boundary conditions at $x = 0$,

$$u_1(0) = 0,$$

and u_2 satisfies the boundary condition at $x = \pi$,

$$u_2(\pi) = 0.$$

Since the Wronskian W of u_1 and u_2 satisfies

$$\begin{aligned} W(y) &= \begin{vmatrix} u_1(y) & u_2(y) \\ u_1'(y) & u_2'(y) \end{vmatrix} \\ &= u_1(y)u_2'(y) - u_2(y)u_1'(y) \\ &= -\sin \sqrt{\lambda} y \sqrt{\lambda} \cos(\sqrt{\lambda} \pi - \sqrt{\lambda} y) - \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} y) \sqrt{\lambda} \cos \sqrt{\lambda} y \\ &= -\sqrt{\lambda} \sin(\sqrt{\lambda} y + \sqrt{\lambda} \pi - \sqrt{\lambda} y) \\ &= -\sqrt{\lambda} \sin \sqrt{\lambda} \pi \neq 0, \text{ for all } y \in [0, \pi], \end{aligned}$$

u_1 and u_2 are linearly independent.

Now define

$$\begin{aligned} g(x, y) &= \begin{cases} C(y)u_1(x)u_2(y), & 0 \leq x \leq y \leq \pi \\ C(y)u_1(y)u_2(x), & 0 \leq y \leq x \leq \pi \end{cases} \\ &= \begin{cases} C(y) \sin \sqrt{\lambda}x \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}y), & 0 \leq x \leq y \leq \pi \\ C(y) \sin \sqrt{\lambda}y \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}x), & 0 \leq y \leq x \leq \pi, \end{cases} \end{aligned} \quad (3.1.31)$$

where

$$\begin{aligned} C(y) &= -\frac{1}{W(y)} \\ &= \frac{1}{\sqrt{\lambda} \sin \sqrt{\lambda}\pi}. \end{aligned}$$

Substituting the value of $C(y)$ in the equation (3.1.31), we get the equation (3.1.30).

Now it remains to show that all the properties of $g(x, y)$ listed in the Definition 3.1.8 are satisfied. Clearly, $g(x, y) = g(y, x)$ and hence g is symmetric. By the equation (3.1.30), it follows that

$$g(0, y) = 0 = g(\pi, y) \quad \text{and} \quad g(x, 0) = 0 = g(x, \pi),$$

which shows that the property 1 of Definition 3.1.8 is satisfied. The function g is obviously continuous on $[0, \pi] \times [0, \pi]$. Differentiating the equation (3.1.30) with respect to x , we get

$$g_x(x, y) = \begin{cases} \frac{\cos \sqrt{\lambda}x \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}y)}{\sin \sqrt{\lambda}\pi}, & 0 \leq x < y \leq \pi \\ -\frac{\sin \sqrt{\lambda}y \cos(\sqrt{\lambda}\pi - \sqrt{\lambda}x)}{\sin \sqrt{\lambda}\pi}, & 0 \leq y < x \leq \pi. \end{cases}$$

Again differentiating the last equation with respect to x , we get

$$g_{xx}(x, y) = \begin{cases} \frac{-\sqrt{\lambda} \sin \sqrt{\lambda}x \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}y)}{\sin \sqrt{\lambda}\pi}, & 0 \leq x < y \leq \pi \\ -\frac{\sqrt{\lambda} \sin \sqrt{\lambda}y \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}x)}{\sin \sqrt{\lambda}\pi}, & 0 \leq y < x \leq \pi. \end{cases}$$

For $x < y$,

$$\begin{aligned} & -g_{xx}(x, y) - \lambda g(x, y) \\ &= \frac{\sqrt{\lambda} \sin \sqrt{\lambda}x \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}y)}{\sin \sqrt{\lambda}\pi} - \frac{\lambda \sin \sqrt{\lambda}x \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}y)}{\sqrt{\lambda} \sin \sqrt{\lambda}\pi} \\ &= 0. \end{aligned}$$

Similarly, for $x > y$,

$$\begin{aligned}
& -g_{xx}(x, y) - \lambda g(x, y) \\
&= \frac{\sqrt{\lambda} \sin \sqrt{\lambda} y \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sin \sqrt{\lambda} \pi} - \frac{\lambda \sin \sqrt{\lambda} y \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} \\
&= 0.
\end{aligned}$$

Thus, the property 2 of Definition 3.1.8 is satisfied. Finally,

$$\begin{aligned}
g_x(y+, y) - g_x(y-, y) &= \lim_{c \rightarrow y+} g_x(c, y) - \lim_{c \rightarrow y-} g_x(c, y) \\
&= \lim_{c \rightarrow y+} \frac{-\sin \sqrt{\lambda} y \cos(\sqrt{\lambda} \pi - \sqrt{\lambda} c)}{\sin \sqrt{\lambda} \pi} \\
&\quad - \lim_{c \rightarrow y-} \frac{\cos \sqrt{\lambda} c \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} y)}{\sin \sqrt{\lambda} \pi} \\
&= \frac{-\sin(\sqrt{\lambda} y + \sqrt{\lambda} \pi - \sqrt{\lambda} y)}{\sin \sqrt{\lambda} \pi} \\
&= -1.
\end{aligned}$$

Therefore, the property 3 of Definition 3.1.8 is also satisfied. \square

In Theorem 3.1.11, we saw that if 0 is not an eigenvalue of H_0 , the resolvent H_0^{-1} exists and is a compact self-adjoint operator. The following theorem is similar to Theorem 3.1.11 where we show that the resolvent $(H_0 - \lambda I)^{-1}$ exists and is a compact self-adjoint operator for any nonzero $\lambda \in \mathbb{R}$ which is not an eigenvalue of H_0 .

Theorem 3.1.13. *Let $\lambda \in \mathbb{R} \setminus \{n^2\}_{n=0}^{\infty}$. Let $L = (H_0 - \lambda I) : \mathcal{D} \mapsto \mathcal{H}$, where \mathcal{D} is defined by the equation (3.1.21), be given by*

$$Lu = -u'' - \lambda u$$

and assume that

$$Lu = 0 \implies u = 0.$$

Let g be the Green function for L given by the equation (3.1.30). Let $G : \mathcal{H} \mapsto \mathcal{H}$ be the integral operator defined by

$$(Gf)(x) = \int_0^\pi g(x, y) f(y) dy. \quad (3.1.32)$$

Then, G is a compact self-adjoint operator on \mathcal{H} , $Gf \in \mathcal{D}$ for all $f \in \mathcal{H}$, $LGf = f$ for all $f \in \mathcal{H}$, and $GLh = h$ for all h in \mathcal{D} .

Proof. The proof that G is a compact self-adjoint operator follows exactly as in Theorem 3.1.11.

Let us fix some $f \in \mathcal{H}$ and let $h = Gf$. We wish to show that $h \in \mathcal{D}$. We have

$$\begin{aligned}
h(x) &= \int_0^\pi g(x, y) f(y) dy \\
&= \int_0^x g(x, y) f(y) dy + \int_x^\pi g(x, y) f(y) dy \\
&= \int_0^x \frac{\sin \sqrt{\lambda} y \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} f(y) dy + \int_x^\pi \frac{\sin \sqrt{\lambda} x \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} y)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} f(y) dy \\
&= \frac{\sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} \int_0^x \sin \sqrt{\lambda} y f(y) dy + \frac{\sin \sqrt{\lambda} x}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} \int_x^\pi \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} y) f(y) dy.
\end{aligned}$$

By the Hölder inequality, we get

$$\int_0^\pi |\sin \sqrt{\lambda} y f(y)| dy \leq \left(\int_0^\pi |\sin \sqrt{\lambda} y|^2 dy \right)^{1/2} \left(\int_0^\pi |f(y)|^2 dy \right)^{1/2} < \infty,$$

which implies that $\sin \sqrt{\lambda} y f(y) \in L^1([0, \pi])$.

Similarly, we can show that $\sin(\sqrt{\lambda} \pi - \sqrt{\lambda} y) f(y) \in L^1([0, \pi])$. Therefore,

$$h_1(x) := \int_0^x \sin \sqrt{\lambda} y f(y) dy$$

and

$$h_2(x) := \int_x^\pi \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} y) f(y) dy$$

are absolutely continuous, and

$$h_1'(x) = \sin \sqrt{\lambda} x f(x) \text{ for almost every } x \in [0, \pi],$$

and

$$h_2'(x) = -\sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x) f(x) \text{ for almost every } x \in [0, \pi].$$

Therefore, we have

$$\begin{aligned}
h'(x) &= \frac{\sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} \sin \sqrt{\lambda} x f(x) - \frac{\sqrt{\lambda} \cos(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} h_1(x) \\
&\quad - \frac{\sin \sqrt{\lambda} x}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} \sin(\sqrt{\lambda} \pi - \sqrt{\lambda} x) f(x) + \frac{\sqrt{\lambda} \cos \sqrt{\lambda} x}{\sqrt{\lambda} \sin \sqrt{\lambda} \pi} h_2(x) \\
&= \frac{\cos \sqrt{\lambda} x}{\sin \sqrt{\lambda} \pi} h_2(x) - \frac{\cos(\sqrt{\lambda} \pi - \sqrt{\lambda} x)}{\sin \sqrt{\lambda} \pi} h_1(x) \text{ for all } x \in [0, \pi], \tag{3.1.33}
\end{aligned}$$

since $\cos \sqrt{\lambda}x$, $h_2(x)$, $\cos(\sqrt{\lambda}\pi - \sqrt{\lambda}x)$, and $h_1(x)$ are all absolutely continuous on $[0, \pi]$. Therefore, $h'(x)$ is also absolutely continuous on $[0, \pi]$. Differentiating the equation (3.1.33), we get

$$\begin{aligned}
h''(x) &= \frac{\cos \sqrt{\lambda}x}{\sin \sqrt{\lambda}\pi} h_2'(x) - \frac{\sqrt{\lambda} \sin \sqrt{\lambda}x}{\sin \sqrt{\lambda}\pi} h_2(x) - \frac{\cos(\sqrt{\lambda}\pi - \sqrt{\lambda}x)}{\sin \sqrt{\lambda}\pi} h_1'(x) \\
&\quad - \frac{\sqrt{\lambda} \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}x)}{\sin \sqrt{\lambda}\pi} h_1(x) \\
&= -\frac{\cos \sqrt{\lambda}x}{\sin \sqrt{\lambda}\pi} \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}x) f(x) - \frac{\sqrt{\lambda} \sin \sqrt{\lambda}x}{\sin \sqrt{\lambda}\pi} h_2(x) \\
&\quad - \frac{\cos(\sqrt{\lambda}\pi - \sqrt{\lambda}x)}{\sin \sqrt{\lambda}\pi} \sin \sqrt{\lambda}x f(x) - \frac{\sqrt{\lambda} \sin(\sqrt{\lambda}\pi - \sqrt{\lambda}x)}{\sin \sqrt{\lambda}\pi} h_1(x) \\
&= -\frac{\sin(\sqrt{\lambda}x + \sqrt{\lambda}\pi - \sqrt{\lambda}x) f(x)}{\sin \sqrt{\lambda}\pi} - \lambda h(x) \\
&= -f(x) - \lambda h(x) \text{ for almost every } x \in [0, \pi].
\end{aligned} \tag{3.1.34}$$

Since both f and h are in \mathcal{H} , h'' is also in \mathcal{H} . Also, $h(0) = 0 = h(\pi)$. Hence, $h \in \mathcal{D}$.

To show $LGf = f$ for all $f \in \mathcal{H}$, let $h = Gf$. Then, $Lh = -h'' - \lambda h = f$ by the equation (3.1.34).

To show $GLh = h$ for all $h \in \mathcal{D}$, let $h \in \mathcal{D}$. Then, $Lh \in \mathcal{H}$. Since $LGf = f$ for all $f \in \mathcal{H}$, $LGLh = Lh$, which implies that $L(GLh - h) = 0$. Since $\ker L = \{0\}$, it follows that $GLh = h$. \square

Lemma 3.1.14. *Let $H_0 : \mathcal{D} \mapsto \mathcal{H}$, where \mathcal{D} is defined by the equation (3.1.21), be given by*

$$H_0 f = -f''. \tag{3.1.35}$$

Then, the eigenvalues of H_0 are $\{n^2\}_{n=1}^{\infty}$ each of multiplicity one. The eigenspace of the eigenvalue n^2 is $\text{span} \{\sin(nx)\}$.

Proof. Let us consider the equation

$$H_0 f = \lambda f \tag{3.1.36}$$

under the boundary conditions

$$f(0) = f(\pi) = 0. \tag{3.1.37}$$

By the equations (3.1.35) and (3.1.36),

$$f'' + \lambda f = 0. \tag{3.1.38}$$

Let us first consider the case where $\lambda > 0$. The general solution of the equation (3.1.38) is given by

$$f(x) = A \cos \sqrt{\lambda}x + B \sin \sqrt{\lambda}x. \quad (3.1.39)$$

Applying the boundary conditions given by the equation (3.1.37), we get

$$0 = f(0) = A \cos 0 + B \sin 0,$$

which gives $A = 0$, and

$$0 = f(\pi) = A \cos \sqrt{\lambda}\pi + B \sin \sqrt{\lambda}\pi.$$

Since $A = 0$, the latter expression becomes $B \sin \sqrt{\lambda}\pi = 0$. If $B = 0$, then by the equation (3.1.39) we will have a trivial solution of the equation (3.1.38) for all $\lambda > 0$, and the trivial solution is not admissible as an eigenfunction. So, we assume $B \neq 0$ and this implies that $\sin \sqrt{\lambda}\pi = 0$. Therefore, we have $\sqrt{\lambda}\pi = n\pi$, $n \in \mathbb{N}$, that is, $\lambda_n = n^2$, $n \in \mathbb{N}$.

If $\lambda = 0$, then $f(x) = A + Bx$ is the general solution of the differential equation (3.1.38). After applying the boundary conditions given by the equation (3.1.37), we get both A and B to be zero, which implies f to be a trivial solution. Therefore, $\lambda = 0$ cannot be an eigenvalue of H_0 .

Let $\lambda < 0$. Then, the general solution of the differential equation (3.1.38) is given by

$$f(x) = c_1 e^{\sqrt{-\lambda}x} + c_2 e^{-\sqrt{-\lambda}x}.$$

Applying the boundary conditions given by the equation (3.1.37), we get $0 = f(0) = c_1 + c_2$, which gives $c_1 = -c_2$, and

$$0 = f(\pi) = c_1 e^{\sqrt{-\lambda}\pi} + c_2 e^{-\sqrt{-\lambda}\pi}.$$

Since $c_1 = -c_2$, the latter expression equals

$$0 = c_1 \left(e^{\sqrt{-\lambda}\pi} - e^{-\sqrt{-\lambda}\pi} \right).$$

Since $\sqrt{-\lambda} > 0$, $e^{\sqrt{-\lambda}\pi} \neq e^{-\sqrt{-\lambda}\pi}$. Therefore, we have $c_1 = c_2 = 0$, which implies f to be a trivial solution. So, $\lambda < 0$ cannot be an eigenvalue of H_0 . Therefore, the eigenvalues of H_0 are $\{n^2\}_{n=1}^{\infty}$ each of multiplicity one and the eigenspace of n^2 is $\text{span} \{\sin(nx)\}$. \square

Lemma 3.1.15. Let $H_0 : \mathcal{D} \mapsto \mathcal{H}$, where \mathcal{D} is defined by the equation (3.1.21), be given by

$$H_0 u = -u''.$$

Then, H_0 is a self-adjoint operator.

Proof. To prove that H_0 is a self-adjoint operator, we must show $H_0 = H_0^*$, where H_0^* is the Hilbert-adjoint of H_0 . We first show that H_0 is symmetric. For $f, g \in \mathcal{D}$,

$$\begin{aligned} \langle H_0 f, g \rangle &= \int_0^\pi (H_0 f) \bar{g} dx \\ &= - \int_0^\pi f'' \bar{g} dx \\ &= -f' \bar{g} \Big|_0^\pi + \int_0^\pi \bar{g}' f' dx \\ &= 0 + \bar{g}' f \Big|_0^\pi - \int_0^\pi \bar{g}'' f dx \\ &= 0 - \int_0^\pi \bar{g}'' f dx \\ &= \langle f, H_0 g \rangle, \end{aligned}$$

which proves that H_0 is symmetric. Since H_0 is symmetric, it follows that $H_0 \subset H_0^*$, that is, $D(H_0) = \mathcal{D} \subset D(H_0^*)$ and $H_0 = H_0^*|_{\mathcal{D}}$. Now, it suffices to show that $H_0^* \subset H_0$. By Lemma 3.1.14, 0 is not an eigenvalue of H_0 and hence by Theorem 3.1.11, the operator G given by the equation (3.1.25), whose domain is all of \mathcal{H} and range \mathcal{D} , is the inverse of H_0 . Therefore, the range of H_0 , denoted by $R(H_0)$, is all of \mathcal{H} , that is, $R(H_0) = \mathcal{H}$. Let $u \in D(H_0^*)$, then $H_0^* u \in \mathcal{H}$. Since $R(H_0) = \mathcal{H}$, there exists some $v \in \mathcal{D}$ such that $H_0^* u = H_0 v$. But $H_0 \subset H_0^*$ implies that $H_0^* v = H_0 v$. Therefore, we have $H_0^* u = H_0^* v$, that is, $H_0^*(u - v) = 0$. Since $N(H_0^*) = R(H_0)^\perp = \{0\}$, $u = v$. Thus, $u \in \mathcal{D}$ and $H_0^* \subset H_0$. \square

Lemma 3.1.16. Let $H_0 : \mathcal{D} \mapsto \mathcal{H}$, where \mathcal{D} is defined by the equation (3.1.21), be given by

$$H_0 u = -u''.$$

Then, the resolvent of H_0 is compact.

Proof. Since the eigenvalues of H_0 are $\{n^2\}_{n=1}^\infty$, for $\lambda \neq n^2$, $(H_0 - \lambda I)u = 0$ implies $u = 0$, for $u \in \mathcal{D}$. If $\lambda = 0$, then by Theorem 3.1.11, it follows that the operator

G given by the equation (3.1.25) is the inverse of H_0 and compact. Thus, H_0^{-1} is a compact operator. If $\lambda \in \mathbb{R} \setminus \{n^2\}_{n=0}^\infty$, then by Theorem 3.1.13, it follows that the operator G given by the equation (3.1.32) is the inverse of $(H_0 - \lambda I)$ and compact. Therefore, $(H_0 - \lambda I)^{-1}$ is a compact operator for all $\lambda \in \mathbb{R} \setminus \{n^2\}_{n=1}^\infty$. Since a compact operator is bounded, and $(H_0 - \lambda I)^{-1}$ exists and compact for all $\lambda \in \mathbb{R} \setminus \{n^2\}_{n=1}^\infty$, it follows that such λ belongs to the resolvent set of H_0 , that is, $\lambda \in \rho(H_0)$. Since H_0 is self-adjoint, $\lambda \in \mathbb{C} \setminus \mathbb{R}$ implies $\lambda \in \rho(H_0)$. Therefore, $\rho(H_0) = \mathbb{C} \setminus \{n^2\}_{n=1}^\infty$. Let $\lambda_0 \in \mathbb{R} \setminus \{n^2\}_{n=1}^\infty$ and $\lambda \in \rho(H_0)$ be such that $\lambda \neq \lambda_0$. By the resolvent identity [17, Theorem VI.5], we have

$$(H_0 - \lambda I)^{-1} = (H_0 - \lambda_0 I)^{-1} + (\lambda - \lambda_0)(H_0 - \lambda I)^{-1}(H_0 - \lambda_0 I)^{-1}. \quad (3.1.40)$$

Since $(H_0 - \lambda I)^{-1}$ is bounded and $(H_0 - \lambda_0 I)^{-1}$ is compact, $(H_0 - \lambda I)^{-1} \cdot (H_0 - \lambda_0 I)^{-1}$ is compact. Therefore, the right hand side of the equation (3.1.40) is compact, and hence $(H_0 - \lambda I)^{-1}$ is compact. Thus, the resolvent of H_0 is compact. \square

Lemma 3.1.17. *Let H_0 , \mathcal{D} , and \mathcal{H} be as in Lemma 3.1.16. Then, the resolvent of H_0 belongs to \mathcal{S}^1 , and, hence, to \mathcal{S}^2 .*

Proof. Let $\mu \in \rho((H_0 - \lambda I)^{-1})$. Then, $((H_0 - \lambda I)^{-1} - \mu I)^{-1}$ is a bounded linear operator. Since

$$(H_0 - \lambda I)^{-1} - \mu I = \mu(\mu^{-1}I - (H_0 - \lambda I))(H_0 - \lambda I)^{-1},$$

it follows that

$$((H_0 - \lambda I)^{-1} - \mu I)^{-1} = (H_0 - \lambda I)(\mu^{-1}I - (H_0 - \lambda I))^{-1}\mu^{-1}.$$

The last expression is equivalent to

$$(H_0 - \lambda I)^{-1}((H_0 - \lambda I)^{-1} - \mu I)^{-1}\mu = (\mu^{-1}I - (H_0 - \lambda I))^{-1}. \quad (3.1.41)$$

Since the left hand side of the equation (3.1.41) is a bounded linear operator, it follows that $(\mu^{-1}I - (H_0 - \lambda I))^{-1} = ((\mu^{-1} + \lambda)I - H_0)^{-1}$ is a bounded linear operator. Since the spectrum of H_0 is $\{n^2\}_{n=1}^\infty$,

$$\mu^{-1} + \lambda \neq n^2, \quad n \in \mathbb{N}.$$

The latter expression is equivalent to

$$\mu \neq \frac{1}{n^2 - \lambda}, \quad n \in \mathbb{N}.$$

Therefore, $\rho((H_0 - \lambda I)^{-1}) \subset \mathbb{C} \setminus \left\{ \frac{1}{n^2 - \lambda} \right\}_{n=1}^{\infty}$. Next, choose $\mu \in \mathbb{C} \setminus \left\{ \frac{1}{n^2 - \lambda} \right\}_{n=1}^{\infty}$. Then, $\mu^{-1} + \lambda \neq n^2$, $n \in \mathbb{N}$. Since the spectrum of H_0 is $\{n^2\}_{n=1}^{\infty}$, it follows that $((\mu^{-1} + \lambda)I - H_0)^{-1} = (\mu^{-1}I - (H_0 - \lambda I))^{-1}$ is a bounded linear operator. By the equation (3.1.41), we conclude that $((H_0 - \lambda I)^{-1} - \mu I)^{-1}$ is a bounded linear operator, which shows that $\mu \in \rho((H_0 - \lambda I)^{-1})$ and hence $\mathbb{C} \setminus \left\{ \frac{1}{n^2 - \lambda} \right\}_{n=1}^{\infty} \subset \rho((H_0 - \lambda I)^{-1})$. Thus, $\rho((H_0 - \lambda I)^{-1}) = \mathbb{C} \setminus \left\{ \frac{1}{n^2 - \lambda} \right\}_{n=1}^{\infty}$ i.e. $\sigma((H_0 - \lambda I)^{-1}) = \left\{ \frac{1}{n^2 - \lambda} \right\}_{n=1}^{\infty}$. Let $\mu_n = \frac{1}{n^2 - \lambda}$, $n \in \mathbb{N}$. Since nonzero points in the spectrum of compact operators are eigenvalues [17, Theorem VI.15] and

$$\sum_{n=1}^{\infty} |\mu_n| < \infty,$$

we conclude that the resolvent of H_0 belong to \mathcal{S}^1 , and, hence to \mathcal{S}^2 . \square

3.2 Commutative Perturbations

In this section, we assume that the initial operator H_0 and its bounded perturbation V commute, that is, $H_0V = VH_0$.

3.2.1 Trace Formulas

Theorem 3.2.1. *Let $H_0 = H_0^*$ satisfy $(I + H_0^2)^{-1/2} \in \mathcal{S}^2$ and let $V = V^* \in \mathcal{B}(\mathcal{H})$. Also, let $H_0V = VH_0$. Then, there is a locally integrable function $\eta_n = \eta_{n, H_0, V}$, $n \geq 3$, with total variation on the segment $[a, b]$*

$$\int_{[a, b]} |\eta_n(\lambda)| d\lambda \leq 2 \cdot C_{a, b} \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \cdot \sum_{k=0}^{n-1} \|V\|^k, \quad (3.2.1)$$

where

$$C_{a, b} = \max_{1 \leq k \leq n-1} \left\{ (b-a)^n \cdot (1 + a^2 + b^2), C_{a, b, k} \cdot (b-a)^{n-1-k} \right\}, \quad n \geq 3,$$

$C_{a, b, k}$ is given by (3.1.6) for $k = 1$ and (3.1.7) for $k \geq 2$, such that

$$\mathrm{Tr} \left(f(H_0 + V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{R}} f^{(n)}(\lambda) \eta_n(\lambda) d\lambda, \quad (3.2.2)$$

for $f \in C_c^n((a, b))$, $a, b \in \mathbb{R}$.

Proof. By Theorem 3.1.7, there is a unique locally finite real-valued measure $\mu_p = \mu_{p,H_0,V}$, $p \geq 3$, with total variation on the segment $[a, b]$

$$\int_{[a,b]} d|\mu_p| \leq 2 \cdot C_{a,b} \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \cdot \sum_{k=0}^{p-1} \|V\|^k,$$

where

$$C_{a,b} = \max_{1 \leq k \leq p-1} \left\{ (b-a)^p \cdot (1 + a^2 + b^2), C_{a,b,k} \cdot (b-a)^{p-1-k} \right\}, \quad p \geq 3,$$

$C_{a,b,k}$ is given by (3.1.6) for $k = 1$ and (3.1.7) for $k \geq 2$, such that

$$\mathrm{Tr}(R_{p,H_0,V}(f)) = \int_{\mathbb{R}} f^{(p)}(\lambda) d\mu_p(\lambda).$$

If $f \in C_c^n((a, b))$, $a, b \in \mathbb{R}$, then $R_{p,H_0,V}(f)$ for $3 \leq p \leq n$ are well defined and

$$\mathrm{Tr}(R_{n,H_0,V}(f)) = \int_{\mathbb{R}} f^{(n)}(\lambda) d\mu_n(\lambda) \quad (3.2.3)$$

and

$$\mathrm{Tr}(R_{n-1,H_0,V}(f)) = \int_{\mathbb{R}} f^{(n-1)}(\lambda) d\mu_{n-1}(\lambda). \quad (3.2.4)$$

By Theorem 2.2.14, we have

$$\begin{aligned} & \left. \frac{d^{n-1}}{dt^{n-1}} \right|_{t=0} f(H_0 + tV) \\ &= (n-1)! \cdot \frac{i^{n-1}}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^{s_0} \dots \int_0^{s_{n-2}} \hat{f}(s_0) e^{i(s_0-s_1)H_0} V \dots V e^{is_{n-1}H_0} ds_{n-1} \dots ds_0. \end{aligned} \quad (3.2.5)$$

Since $H_0V = VH_0$, by spectral theorem, it follows that

$$e^{iH_0t}V = Ve^{iH_0t}, \quad \text{for all } t \in \mathbb{R}. \quad (3.2.6)$$

Using (3.2.6), (3.2.5) becomes

$$\begin{aligned} & \left. \frac{d^{n-1}}{dt^{n-1}} \right|_{t=0} f(H_0 + tV) \\ &= (n-1)! \cdot \frac{i^{n-1}}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_0^{s_0} \dots \int_0^{s_{n-2}} V^{n-1} \hat{f}(s_0) e^{is_0H_0} ds_{n-1} \dots ds_0 \\ &= (n-1)! \cdot \frac{i^{n-1}}{\sqrt{2\pi}} \cdot \frac{V^{n-1}}{(n-1)!} \int_{\mathbb{R}} s_0^{n-1} \hat{f}(s_0) e^{is_0H_0} ds_0 \\ &= \frac{V^{n-1}}{\sqrt{2\pi}} \int_{\mathbb{R}} (is_0)^{n-1} \hat{f}(s_0) e^{is_0H_0} ds_0 \\ &= \frac{V^{n-1}}{\sqrt{2\pi}} \int_{\mathbb{R}} \widehat{f^{(n-1)}}(s_0) e^{is_0H_0} ds_0 \\ &= V^{n-1} f^{(n-1)}(H_0), \end{aligned} \quad (3.2.7)$$

where the last equality follows from Lemma 2.2.13. Since $f^{(n-1)}$ is a continuous compactly supported function on \mathbb{R} , by Lemma 3.1.1 it follows that $f^{(n-1)}(H_0) \in \mathcal{S}^1$ and

$$\begin{aligned} \|f^{(n-1)}(H_0)\|_1 &\leq \|f^{(n-1)}\|_\infty \cdot \left(1 + \max_{s \in \text{supp} f \subset (a,b)} |s|^2\right) \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \\ &\leq \|f^{(n-1)}\|_\infty \cdot (1 + a^2 + b^2) \cdot \|(I + H_0^2)^{-1/2}\|_2^2. \end{aligned}$$

Since $V^{n-1} \in \mathcal{B}(\mathcal{H})$ and \mathcal{S}^1 is a $*$ -ideal in $\mathcal{B}(\mathcal{H})$, it follows that $V^{n-1}f^{(n-1)}(H_0) \in \mathcal{S}^1$ and

$$\|V^{n-1}f^{(n-1)}(H_0)\|_1 \leq \|V\|^{n-1} \cdot \|f^{(n-1)}\|_\infty \cdot (1 + a^2 + b^2) \cdot \|(I + H_0^2)^{-1/2}\|_2^2. \quad (3.2.8)$$

From (3.2.7) and (3.2.8), we see that $\frac{1}{(n-1)!} \frac{d^{n-1}}{dt^{n-1}} \Big|_{t=0} f(H_0 + tV) \in \mathcal{S}^1$ and

$$\begin{aligned} &\frac{1}{(n-1)!} \left| \text{Tr} \left(\frac{d^{n-1}}{dt^{n-1}} \Big|_{t=0} f(H_0 + tV) \right) \right| \\ &\leq \frac{1}{(n-1)!} \left\| \frac{d^{n-1}}{dt^{n-1}} \Big|_{t=0} f(H_0 + tV) \right\|_1 \\ &\leq \frac{1}{(n-1)!} \cdot \|V\|^{n-1} \cdot \|f^{(n-1)}\|_\infty \cdot (1 + a^2 + b^2) \cdot \|(I + H_0^2)^{-1/2}\|_2^2. \end{aligned}$$

Hence, by the Riesz representation theorem for a functional in $(C_c(\mathbb{R}))^*$, there is a unique locally finite real-valued measure $\nu_{n-1} := \nu_{n-1, H_0, V}$ with total variation on the segment $[a, b]$

$$\int_{[a,b]} d|\nu_{n-1}| \leq \frac{(1 + a^2 + b^2)}{(n-1)!} \cdot \|(I + H_0^2)^{-1/2}\|_2^2 \cdot \|V\|^{n-1},$$

such that

$$\frac{1}{(n-1)!} \text{Tr} \left(\frac{d^{n-1}}{dt^{n-1}} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{R}} f^{(n-1)}(\lambda) d\nu_{n-1}(\lambda). \quad (3.2.9)$$

Since ν_{n-1} is finite real-valued measure on \mathbb{R} , the function $F_{\nu_{n-1}} : \mathbb{R} \mapsto \mathbb{R}$ defined by

$$F_{\nu_{n-1}}(\lambda) := \nu_{n-1}((-\infty, \lambda])$$

is a distribution function of ν_{n-1} and

$$\begin{aligned} \int_{\mathbb{R}} f^{(n-1)}(\lambda) d\nu_{n-1}(\lambda) &= \int_{\mathbb{R}} f^{(n-1)}(\lambda) dF_{\nu_{n-1}}(\lambda) \\ &\text{(by parts)} = - \int_{\mathbb{R}} f^{(n)}(\lambda) \nu_{n-1}((-\infty, \lambda]) d\lambda. \end{aligned}$$

Using the last equality, (3.2.9) becomes

$$\frac{1}{(n-1)!} \operatorname{Tr} \left(\left. \frac{d^{n-1}}{dt^{n-1}} \right|_{t=0} f(H_0 + tV) \right) = - \int_{\mathbb{R}} f^{(n)}(\lambda) \nu_{n-1}((-\infty, \lambda]) d\lambda. \quad (3.2.10)$$

Similarly, from (3.2.4), we get

$$\operatorname{Tr}(R_{n-1, H_0, V}(f)) = \int_{\mathbb{R}} f^{(n-1)}(\lambda) d\mu_{n-1}(\lambda) = - \int_{\mathbb{R}} f^{(n)}(\lambda) \mu_{n-1}((-\infty, \lambda]) d\lambda. \quad (3.2.11)$$

Using (3.2.10) and (3.2.11), we get

$$\begin{aligned} \operatorname{Tr}(R_{n, H_0, V}(f)) &= \operatorname{Tr}(R_{n-1, H_0, V}(f)) - \frac{1}{(n-1)!} \operatorname{Tr} \left(\left. \frac{d^{n-1}}{dt^{n-1}} \right|_{t=0} f(H_0 + tV) \right) \\ &= \int_{\mathbb{R}} f^{(n)}(\lambda) (\nu_{n-1}((-\infty, \lambda]) - \mu_{n-1}((-\infty, \lambda])) d\lambda. \end{aligned} \quad (3.2.12)$$

From (3.2.3) and (3.2.12), we have

$$\int_{\mathbb{R}} f^{(n)}(\lambda) d\mu_n(\lambda) = \int_{\mathbb{R}} f^{(n)}(\lambda) (\nu_{n-1}((-\infty, \lambda]) - \mu_{n-1}((-\infty, \lambda])) d\lambda,$$

which along with the uniqueness of μ_n implies that μ_n is absolutely continuous and its density equals

$$\eta_n(\lambda) = \mu_{n-1}((-\infty, \lambda]) - \nu_{n-1}((-\infty, \lambda]).$$

Thus, η_n satisfies (3.2.2). (3.2.1) follows from (3.1.15). □

3.2.2 The case of a Laplacian perturbed by multiplication by a constant

In this section, we will give an example of a Hilbert space \mathcal{H} , a self-adjoint operator H_0 with Hilbert-Schmidt resolvent, and a bounded self-adjoint perturbation V to which Theorem 3.2.1 applies in the cases when $n = 1$ and $n = 2$. We consider the same \mathcal{H} and H_0 as in Section 3.1.1 and define V as in (3.2.13). We first prove that V is a bounded self-adjoint operator on \mathcal{H} (see Lemma 3.2.2). The fact that H_0 has a compact resolvent (see Lemma 3.1.16) will ultimately help us to find the spectral representation for $f(H_0 + tV)$, $t \in \mathbb{R}$ (see Corollary 3.2.6) so that we can compute the expression on the left hand side of (3.2.2). Finally, we find the locally integrable functions $\xi = \eta_{1, H_0, V}$ (see (3.2.20)) and $\eta = \eta_{2, H_0, V}$ (see (3.2.27)) and prove the main

results in Lemma 3.2.9 (case $n = 1$) and Lemma 3.2.10 (case $n = 2$), respectively. In Lemmas 3.2.12 and 3.2.13, we generalize the example to more general class of functions, that is, to the Schwartz class functions.

Let $V : \mathcal{H} \mapsto \mathcal{H}$ be defined by

$$(Vf)(x) = cf(x), \tag{3.2.13}$$

where $c \in \mathbb{R}$. Clearly, the operator V is bounded. The lemma below shows that the operator V is self-adjoint.

Lemma 3.2.2. *Let $V : \mathcal{H} \mapsto \mathcal{H}$ be defined by the equation (3.2.13). Then, V is self-adjoint.*

Proof. For $f, g \in \mathcal{H}$,

$$\begin{aligned} \langle Vf, g \rangle &= \int_0^\pi (Vf)\bar{g}dx \\ &= \int_0^\pi (cf)\bar{g}dx \\ &= \int_0^\pi f\bar{c}gdx \\ &= \langle f, Vg \rangle, \end{aligned}$$

which proves that V is self-adjoint. □

We need the following theorem to give the spectral representation for H_0 .

Theorem 3.2.3. *(See [17, Theorem VI.16]) Let T be a compact self-adjoint operator on a Hilbert space \mathcal{H} . Then, there is a complete orthonormal basis, $\{\phi_n\}_{n=1}^\infty$, for \mathcal{H} so that $T\phi_n = \lambda_n\phi_n$ and $\lambda_n \rightarrow 0$ as $n \rightarrow \infty$.*

Lemma 3.2.4. *Let H_0 be defined by the equation (3.1.22). Then, the spectral representation of H_0 is given by*

$$H_0 = \sum_{n=1}^{\infty} n^2 P_{n^2},$$

where

$$P_{n^2} = \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx).$$

Proof. Since H_0^{-1} is a compact self-adjoint operator with eigenvalues $\left\{\frac{1}{n^2}\right\}_{n=1}^{\infty}$, by Theorem 3.2.3, there is a complete orthonormal basis $\{\psi_n\}$ for \mathcal{H} so that

$$H_0^{-1}\psi_n = \frac{1}{n^2}\psi_n, \quad \frac{1}{n^2} \rightarrow 0 \text{ as } n \rightarrow \infty.$$

The latter expression is equivalent to

$$H_0\psi_n = n^2\psi_n, \quad n \in \mathbb{N}.$$

By Lemma 3.1.14, we have

$$H_0 \sin(nx) = n^2 \sin(nx), \quad n \in \mathbb{N},$$

and the multiplicity of n^2 is one. Therefore, $\psi_n = \alpha \cdot \sin(nx)$ for some scalar α . In particular, we take $\psi_n = \frac{\sin(nx)}{\sqrt{\pi/2}}$, $n \in \mathbb{N}$ so that $\left\{\frac{\sin(nx)}{\sqrt{\pi/2}}\right\}_{n=1}^{\infty}$ is a complete orthonormal basis for \mathcal{H} . Let $f \in \mathcal{D} \subset \mathcal{H}$, then

$$f(x) = \sum_{n=1}^{\infty} a_n \frac{\sin(nx)}{\sqrt{\pi/2}},$$

where

$$a_n = \left\langle f(x), \frac{\sin(nx)}{\sqrt{\pi/2}} \right\rangle = \sqrt{\frac{2}{\pi}} \int_0^{\pi} f(x) \sin(nx) dx.$$

Similarly, we have

$$g(x) := H_0 f(x) = \sum_{n=1}^{\infty} b_n \frac{\sin(nx)}{\sqrt{\pi/2}},$$

where

$$b_n = \left\langle g(x), \frac{\sin(nx)}{\sqrt{\pi/2}} \right\rangle = \sqrt{\frac{2}{\pi}} \int_0^{\pi} g(x) \sin(nx) dx.$$

Since

$$\begin{aligned} b_n &= \left\langle g(x), \frac{\sin(nx)}{\sqrt{\pi/2}} \right\rangle = \left\langle H_0 f(x), \frac{\sin(nx)}{\sqrt{\pi/2}} \right\rangle = \left\langle f(x), \frac{H_0 \sin(nx)}{\sqrt{\pi/2}} \right\rangle \\ &= \left\langle f(x), \frac{n^2 \sin(nx)}{\sqrt{\pi/2}} \right\rangle = n^2 \left\langle f(x), \frac{\sin(nx)}{\sqrt{\pi/2}} \right\rangle = n^2 a_n, \end{aligned}$$

we have the following representation

$$H_0 f(x) = \sum_{n=1}^{\infty} n^2 a_n \frac{\sin(nx)}{\sqrt{\pi/2}}. \quad (3.2.14)$$

If we define an operator $P_{n^2} : \mathcal{H} \mapsto \mathcal{H}$ by $(P_{n^2} f)(x) = \sqrt{\frac{2}{\pi}} a_n \sin(nx)$, then clearly P_{n^2} is the orthogonal projection of \mathcal{H} onto the eigenspace of H_0 corresponding to n^2 . Therefore, the equation (3.2.14) can be written as

$$H_0 f(x) = \sum_{n=1}^{\infty} n^2 P_{n^2} f(x), \quad (3.2.15)$$

completing the proof of the lemma. \square

Lemma 3.2.5. *Let H_0 and V be defined by (3.1.22) and (3.2.13), respectively. Then, for any $t \in \mathbb{R}$, the spectral representation of $H_0 + tV$ is given by*

$$H_0 + tV = \sum_{n=1}^{\infty} (ct + n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx). \quad (3.2.16)$$

Proof. Since $H_0 = H_0^*$ has compact resolvent and $V = V^*$ is a bounded operator, by [2, Lemma 1.3] $H_0 + tV$, for $t \in \mathbb{R}$, also has compact resolvent. Since the eigenvalues of $H_0 + tV$ are $\{ct + n^2\}_{n=1}^{\infty}$ each of multiplicity one and eigenspace of $(ct + n^2)$ is $\text{span} \{\sin(nx)\}$, the proof exactly follows as in the case of H_0 . \square

Corollary 3.2.6. *For $f \in C_c^3(\mathbb{R})$ and $t \in \mathbb{R}$, the spectral representation of $f(H_0 + tV)$ is given by*

$$f(H_0 + tV) = \sum_{n=1}^{\infty} f(ct + n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx). \quad (3.2.17)$$

For $t = 0$ and $t = 1$, we have from Corollary 3.2.6

$$f(H_0) = \sum_{n=1}^{\infty} f(n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx) \quad (3.2.18)$$

and

$$f(H_0 + V) = \sum_{n=1}^{\infty} f(c + n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx), \quad (3.2.19)$$

respectively.

Remark 3.2.7. *Since any compact subset δ of \mathbb{R} contains finitely many eigenvalues of $H_0 + tV$, $t \in [0, 1]$, it follows that the spectral measure $E_{H_0+tV}(\delta)$ has a finite rank, and $\text{Tr}(E_{H_0+tV}(\delta))$ equals the number of eigenvalues of $H_0 + tV$ in the set δ .*

Lemma 3.2.8. *Let H_0 and V be defined by (3.1.22) and (3.2.13), respectively. For $a < 1$, let*

$$\xi(\lambda) := \text{Tr}\left(E_{H_0}((a, \lambda]) - E_{H_0+V}((a, \lambda])\right).$$

Then for $0 < c < 3$, we have

$$\xi(\lambda) = \begin{cases} 0 & \text{if } a < \lambda < 1 \\ 1 & \text{if } n^2 \leq \lambda < c + n^2 \\ 0 & \text{if } c + n^2 \leq \lambda < (n + 1)^2, \end{cases} \quad (3.2.20)$$

for $n \in \mathbb{N}$.

Proof. The proof directly follows from Remark 3.2.7. □

The following two lemmas demonstrate the results of [2, Theorem 2.5] and [18, Theorem 3.10], respectively, for a specific choice of \mathcal{H} , H_0 , and V . Moreover, the method of our proof is purely computational and does not rely on the proof given in [2, Theorem 2.5] and [18, Theorem 3.10].

Lemma 3.2.9. *Let H_0 and V be as in the equations (3.1.22) and (3.2.13), respectively and $0 < c < 3$. Let $f \in C_c^3((a, b))$, $a, b \in \mathbb{R}$ and $a < 1$. Then,*

$$\text{Tr}(f(H_0 + V)) - \text{Tr}(f(H_0)) = \int_{\mathbb{R}} f'(\lambda) \xi(\lambda) d\lambda,$$

where $\xi(\lambda)$ is given by the equation (3.2.20).

Proof. Since $f \in C_c^3((a, b))$, $a, b \in \mathbb{R}$ and $a < 1$, both the sums given by the equations (3.2.18) and (3.2.19) are finite sums. Therefore, the operators $f(H_0)$ and $f(H_0 + V)$ are finite rank operators, and hence trace class operators. Using the equations (3.2.18) and (3.2.19), we have

$$\begin{aligned} \text{Tr}(f(H_0 + V)) - \text{Tr}(f(H_0)) &= \text{Tr}\left(\sum_{n=1}^{\infty} f(c + n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx)\right) \\ &\quad - \text{Tr}\left(\sum_{n=1}^{\infty} f(n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx)\right) \end{aligned}$$

$$\begin{aligned}
&= \sum_{n=1}^{\infty} f(c+n^2) \operatorname{Tr} \left(\frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx) \right) \\
&\quad - \sum_{n=1}^{\infty} f(n^2) \operatorname{Tr} \left(\frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx) \right) \\
&= \sum_{n=1}^{\infty} f(c+n^2) - \sum_{n=1}^{\infty} f(n^2) \\
&= \sum_{n=1}^{\infty} \left(f(c+n^2) - f(n^2) \right). \tag{3.2.21}
\end{aligned}$$

Now using the equation (3.2.20), we have

$$\begin{aligned}
\int_{\mathbb{R}} f'(\lambda) \xi(\lambda) d\lambda &= \int_{(a,1)} f'(\lambda) \xi(\lambda) d\lambda + \int_{[1,c+1)} f'(\lambda) \xi(\lambda) d\lambda + \int_{[c+1,4)} f'(\lambda) \xi(\lambda) d\lambda \\
&\quad + \int_{[4,c+4)} f'(\lambda) \xi(\lambda) d\lambda + \int_{[c+4,9)} f'(\lambda) \xi(\lambda) d\lambda + \int_{[9,c+9)} f'(\lambda) \xi(\lambda) d\lambda \\
&\quad + \dots + \int_{[n^2,c+n^2)} f'(\lambda) \xi(\lambda) d\lambda + \int_{[c+n^2,(n+1)^2)} f'(\lambda) \xi(\lambda) d\lambda + \dots \\
&= 0 + \int_{[1,c+1)} f'(\lambda) d\lambda + 0 + \int_{[4,c+4)} f'(\lambda) d\lambda + 0 + \int_{[9,c+9)} f'(\lambda) d\lambda + 0 \\
&\quad + \dots + 0 + \int_{[n^2,c+n^2)} f'(\lambda) d\lambda + 0 + \dots \\
&= f(c+1) - f(1) + f(c+4) - f(4) + f(c+9) - f(9) \\
&\quad + \dots + f(c+n^2) - f(n^2) + \dots \\
&= \sum_{n=1}^{\infty} \left(f(c+n^2) - f(n^2) \right). \tag{3.2.22}
\end{aligned}$$

Combining the equations (3.2.21) and (3.2.22) completes the proof of the lemma. \square

Lemma 3.2.10. *Let H_0 and V be as in the equations (3.1.22) and (3.2.13), respectively and $0 < c < 3$. Let $f \in C_c^3((a, b))$, $a, b \in \mathbb{R}$ and $a < 1$. Then,*

$$\operatorname{Tr}(f(H_0 + tV) - f(H_0) - \frac{d}{dt} \Big|_{t=0} f(H_0 + tV)) = \int_{\mathbb{R}} f''(\lambda) \eta(\lambda) d\lambda,$$

where

$$\eta(\lambda) = \mu((a, \lambda]) - \int_a^\lambda \xi(t) dt, \tag{3.2.23}$$

μ is a locally finite measure on \mathbb{R} given by the equation (3.2.26) and ξ is given by the equation (3.2.20).

Proof. Using the fact that $f \in C_c^3((a, b))$, $a, b \in \mathbb{R}$ and $a < 1$, we have from the equations (3.2.17) and (3.2.18)

$$\begin{aligned}
\left. \frac{d}{dt} \right|_{t=0} f(H_0 + tV) &= \lim_{t \rightarrow 0} \frac{f(H_0 + tV) - f(H_0)}{t} \\
&= \lim_{t \rightarrow 0} \frac{1}{t} \left(\sum_{n=1}^{\infty} f(ct + n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx) \right. \\
&\quad \left. - \sum_{n=1}^{\infty} f(n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx) \right) \\
&= \sum_{n=1}^{\infty} \lim_{t \rightarrow 0} \frac{f(ct + n^2) - f(n^2)}{t} \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx) \\
&= \sum_{n=1}^{\infty} cf'(n^2) \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx), \tag{3.2.24}
\end{aligned}$$

and the latter sum is a finite sum. Thus, $\left. \frac{d}{dt} \right|_{t=0} f(H_0 + tV)$ is a finite rank operator and hence a trace class operator. Taking the trace on both sides of the equation (3.2.24), we get

$$\text{Tr} \left(\left. \frac{d}{dt} \right|_{t=0} f(H_0 + tV) \right) = \sum_{n=1}^{\infty} cf'(n^2). \tag{3.2.25}$$

Let A be a subset of \mathbb{R} and define

$$\delta_{n^2}(A) = \begin{cases} 1 & \text{if } n^2 \in A \\ 0 & \text{if } n^2 \notin A \end{cases}$$

and

$$\mu(A) = \sum_{n=1}^{\infty} c \delta_{n^2}(A).$$

Then, μ is a locally finite measure on \mathbb{R} . For $0 < c < 3$ and $a < 1$, the measure μ satisfies

$$\mu((a, \lambda]) = \begin{cases} 0 & \text{if } a < \lambda < 1 \\ nc & \text{if } n^2 \leq \lambda < c + n^2 \\ nc & \text{if } c + n^2 \leq \lambda < (n+1)^2, \end{cases} \tag{3.2.26}$$

for $n \in \mathbb{N}$.

Let ξ be as in the equation (3.2.20). Then, for $a < \lambda < 1$,

$$\int_a^\lambda \xi(t) dt = \int_a^\lambda 0 dt = 0.$$

For $1 \leq \lambda < c + 1$,

$$\int_a^\lambda \xi(t) dt = \int_{(a,1)} \xi(t) dt + \int_{[1,\lambda]} \xi(t) dt = 0 + (\lambda - 1) = \lambda - 1.$$

For $c + 1 \leq \lambda < 4$,

$$\int_a^\lambda \xi(t) dt = \int_{(a,1)} \xi(t) dt + \int_{[1,c+1]} \xi(t) dt + \int_{[c+1,\lambda]} \xi(t) dt = 0 + (c + 1 - 1) + 0 = c.$$

For $4 \leq \lambda < c + 4$,

$$\begin{aligned} \int_a^\lambda \xi(t) dt &= \int_{(a,1)} \xi(t) dt + \int_{[1,c+1]} \xi(t) dt + \int_{[c+1,4]} \xi(t) dt + \int_{[4,\lambda]} \xi(t) dt \\ &= 0 + (c + 1 - 1) + 0 + (\lambda - 4) = c + \lambda - 4. \end{aligned}$$

For $c + 4 \leq \lambda < 9$,

$$\begin{aligned} &\int_a^\lambda \xi(t) dt \\ &= \int_{(a,1)} \xi(t) dt + \int_{[1,c+1]} \xi(t) dt + \int_{[c+1,4]} \xi(t) dt + \int_{[4,c+4]} \xi(t) dt + \int_{[c+4,\lambda]} \xi(t) dt \\ &= 0 + (c + 1 - 1) + 0 + (c + 4 - 4) + 0 = 2c. \end{aligned}$$

Therefore, in general, we have

$$\int_a^\lambda \xi(t) dt = \begin{cases} 0 & \text{if } a < \lambda < 1 \\ (n - 1)c + \lambda - n^2 & \text{if } n^2 \leq \lambda < c + n^2 \\ nc & \text{if } c + n^2 \leq \lambda < (n + 1)^2, \end{cases}$$

for $n \in \mathbb{N}$.

Thus, we have

$$\begin{aligned} \eta(\lambda) &= \mu((a, \lambda]) - \int_a^\lambda \xi(t) dt \\ &= \begin{cases} 0 & \text{if } a < \lambda < 1 \\ c + n^2 - \lambda & \text{if } n^2 \leq \lambda < c + n^2 \\ 0 & \text{if } c + n^2 \leq \lambda < (n + 1)^2, \end{cases} \end{aligned} \quad (3.2.27)$$

for $n \in \mathbb{N}$.

Now using the equation (3.2.27), we get

$$\begin{aligned} \int_{\mathbb{R}} f''(\lambda) \eta(\lambda) d\lambda &= \left(\int_{(a,1)} + \int_{[1,c+1]} + \int_{[c+1,4]} + \int_{[4,c+4]} + \dots + \int_{[n^2,c+n^2]} \right. \\ &\quad \left. + \int_{[c+n^2,(n+1)^2]} + \dots \right) f''(\lambda) \eta(\lambda) d\lambda \end{aligned}$$

$$\begin{aligned}
&= \int_{[1,c+1]} f''(\lambda)(c+1-\lambda)d\lambda + \int_{[4,c+4]} f''(\lambda)(c+4-\lambda)d\lambda + \dots \\
&\quad + \int_{[n^2,c+n^2]} f''(\lambda)(c+n^2-\lambda)d\lambda + \dots
\end{aligned}$$

Integrating by parts, we obtain

$$\begin{aligned}
&\int_{\mathbb{R}} f''(\lambda)\eta(\lambda)d\lambda \\
&= (c+1-\lambda)f'(\lambda)\Big|_1^{c+1} + \int_{[1,c+1]} f'(\lambda)d\lambda + (c+4-\lambda)f'(\lambda)\Big|_4^{c+4} \\
&\quad + \int_{[4,c+4]} f'(\lambda)d\lambda + \dots + (c+n^2-\lambda)f'(\lambda)\Big|_{n^2}^{c+n^2} + \int_{[n^2,c+n^2]} f'(\lambda)d\lambda + \dots \\
&= -cf'(1) + f(c+1) - f(1) - cf'(4) + f(c+4) - f(4) - \dots \\
&\quad - cf'(n^2) + f(c+n^2) - f(n^2) - \dots \\
&= \sum_{n=1}^{\infty} \left(f(c+n^2) - f(n^2) - cf'(n^2) \right). \tag{3.2.28}
\end{aligned}$$

Combination of the equations (3.2.21), (3.2.25), and (3.2.28), concludes the proof of the lemma.

Remark 3.2.11. *A formula similar to (3.2.23) holds in the case of arbitrary $H_0 = H_0^*$ (without restrictions on the resolvent of H_0) and $V = V^* \in \mathcal{S}^1$ (see [10]).*

□

Lemma 3.2.12. *Let H_0 and V be as in the equations (3.1.22) and (3.2.13), respectively, and $0 < c < 3$. Let $f \in \mathcal{S}(\mathbb{R})$, where $\mathcal{S}(\mathbb{R})$ denotes the set of all Schwartz functions on \mathbb{R} . Then,*

$$\mathrm{Tr}(f(H_0 + V)) - \mathrm{Tr}(f(H_0)) = \int_{\mathbb{R}} f'(\lambda)\xi(\lambda)d\lambda,$$

where ξ is as in Lemma 3.2.8 with $a \in \mathbb{R}$ replaced by $-\infty$.

Proof. Since $f \in \mathcal{S}(\mathbb{R})$, there exists $M_{k,l} > 0$ such that

$$\sup_{x \in \mathbb{R}} |x|^k |f^{(l)}(x)| \leq M_{k,l},$$

for all integers $k, l \geq 0$. In particular, for $x = n^2$, $n \in \mathbb{N}$, and $k = 1$ we have

$$|f^{(l)}(n^2)| \leq \frac{M_l}{n^2},$$

for all integers $l \geq 0$. Since $\sum_{n=1}^{\infty} \frac{M_l}{n^2} < \infty$, we have

$$\sum_{n=1}^{\infty} |f^{(l)}(n^2)| < \infty, \quad (3.2.29)$$

for all integers $l \geq 0$. By Lemma 3.2.5, we have

$$H_0 + tV = \sum_{n=1}^{\infty} (ct + n^2)P_{n^2},$$

where

$$P_{n^2} = \frac{2}{\pi} \langle \cdot, \sin(nx) \rangle \sin(nx).$$

Since $f \in \mathcal{S}(\mathbb{R})$, it is bounded and continuous on \mathbb{R} . Therefore by functional calculus (see [Appendix, Section 4.3.5]), we have

$$f(H_0 + tV) = \sum_{n=1}^{\infty} f(ct + n^2)P_{n^2}. \quad (3.2.30)$$

In particular, when $t = 0$ and $t = 1$, we have

$$f(H_0) = \sum_{n=1}^{\infty} f(n^2)P_{n^2}. \quad (3.2.31)$$

and

$$f(H_0 + V) = \sum_{n=1}^{\infty} f(c + n^2)P_{n^2}.$$

From the inequality (3.2.29), we have $\sum_{n=1}^{\infty} |f(n^2)| < \infty$. Similarly, it follows that

$\sum_{n=1}^{\infty} |f(c + n^2)| < \infty$. Therefore, both $f(H_0)$ and $f(H_0 + V)$ are trace class operators, and

$$\mathrm{Tr}(f(H_0)) = \sum_{n=1}^{\infty} f(n^2) \quad (3.2.32)$$

and

$$\mathrm{Tr}(f(H_0 + V)) = \sum_{n=1}^{\infty} f(c + n^2). \quad (3.2.33)$$

From the equations (3.2.32) and (3.2.33), we get

$$\mathrm{Tr}\left(f(H_0 + V) - f(H_0)\right) = \sum_{n=1}^{\infty} \left(f(c + n^2) - f(n^2)\right). \quad (3.2.34)$$

If we proceed exactly as in Lemma 3.2.9, we get

$$\int_{\mathbb{R}} f'(\lambda)\xi(\lambda)d\lambda = \sum_{n=1}^{\infty} \left(f(c + n^2) - f(n^2)\right). \quad (3.2.35)$$

Combining the equations (3.2.34) and (3.2.35) completes the proof of the lemma. \square

Lemma 3.2.13. *Let H_0 and V be as in the equations (3.1.22) and (3.2.13), respectively, and $0 < c < 3$. Let $f \in \mathcal{S}(\mathbb{R})$, where $\mathcal{S}(\mathbb{R})$ denotes the set of all Schwartz functions on \mathbb{R} . Then,*

$$\mathrm{Tr}\left(f(H_0 + tV) - f(H_0) - \frac{d}{dt}\Big|_{t=0} f(H_0 + tV)\right) = \int_{\mathbb{R}} f''(\lambda)\eta(\lambda)d\lambda,$$

where η is as in Lemma 3.2.10 with $a \in \mathbb{R}$ replaced by $-\infty$.

Proof. Using the equations (3.2.30) and (3.2.31), we have

$$\begin{aligned} \frac{d}{dt}\Big|_{t=0} f(H_0 + tV) &= \lim_{t \rightarrow 0} \frac{f(H_0 + tV) - f(H_0)}{t} \\ &= \lim_{t \rightarrow 0} \frac{1}{t} \left(\sum_{n=1}^{\infty} f(ct + n^2)P_{n^2} - \sum_{n=1}^{\infty} f(n^2)P_{n^2} \right) \\ &= \lim_{t \rightarrow 0} \sum_{n=1}^{\infty} \frac{f(ct + n^2) - f(n^2)}{t} P_{n^2}. \end{aligned} \quad (3.2.36)$$

Since $\|P_{n^2}\| = 1$, by the Mean Value Theorem, for all $t \in (0, 1)$, we have

$$\left\| \frac{f(ct + n^2) - f(n^2)}{t} P_{n^2} \right\| = \left| \frac{f(ct + n^2) - f(n^2)}{t} \right| = c|f'(m_{n^2})|, \quad m_{n^2} \in (n^2, ct + n^2).$$

From the equation (3.2.29), it follows that $\sum_{n=1}^{\infty} c|f'(m_{n^2})| < \infty$. Therefore by the Weierstrass M-test for a series of functions with values in a Banach space,

$\sum_{n=1}^{\infty} \frac{f(ct + n^2) - f(n^2)}{t} P_{n^2}$ converges uniformly in $t \in (0, 1)$. Therefore, the equation (3.2.36) becomes

$$\begin{aligned} \frac{d}{dt}\Big|_{t=0} f(H_0 + tV) &= \sum_{n=1}^{\infty} \lim_{t \rightarrow 0} \frac{f(ct + n^2) - f(n^2)}{t} P_{n^2} \\ &= \sum_{n=1}^{\infty} c f'(n^2) P_{n^2}. \end{aligned}$$

Since $\sum_{n=1}^{\infty} c|f'(n^2)| < \infty$, $\frac{d}{dt}\Big|_{t=0} f(H_0 + tV)$ is a trace class operator and

$$\mathrm{Tr}\left(\frac{d}{dt}\Big|_{t=0} f(H_0 + tV)\right) = \sum_{n=1}^{\infty} cf'(n^2). \quad (3.2.37)$$

Combining (3.2.32), (3.2.33), and (3.2.37), we have

$$\mathrm{Tr}\left(f(H_0 + V) - f(H_0) - \frac{d}{dt}\Big|_{t=0} f(H_0 + tV)\right) = \sum_{n=1}^{\infty} \left(f(c + n^2) - f(n^2) - cf'(n^2)\right). \quad (3.2.38)$$

If we proceed exactly as in Lemma 3.2.10, we get

$$\int_{\mathbb{R}} f''(\lambda)\eta(\lambda)d\lambda = \sum_{n=1}^{\infty} \left(f(c + n^2) - f(n^2) - cf'(n^2)\right). \quad (3.2.39)$$

Combining the equations (3.2.38) and (3.2.39) completes the proof of the lemma. \square

Chapter 4

Appendix

4.1 Compact Operators

In this section, we discuss compact operators and its classes. We refer the reader to [4] and [17] for more details.

Definition 4.1.1. [17, Chapter VI, Section 5] A bounded linear operator $T : \mathcal{H} \mapsto \mathcal{H}$ is called compact if for every bounded subset B of \mathcal{H} , the image $T(B)$ is relatively compact, i.e., the closure $\overline{T(B)}$ is compact.

We denote the set of all compact operators on \mathcal{H} by $\mathcal{K}(\mathcal{H})$.

Theorem 4.1.2. [4, Theorem 3.9.4] Let $T \in \mathcal{K}(\mathcal{H})$. Then every nonzero $\lambda \in \sigma(T)$ is an eigenvalue of T and the set of eigenvalues of T is countable with 0 only the possible point of accumulation of that set. If the dimension of \mathcal{H} is infinite, then $\sigma(T)$ contains 0.

Definition 4.1.3. [4, Chapter 11, Section 4] The Schatten-von Neumann ideal of compact operators denoted by \mathcal{S}^p are defined by

$$\mathcal{S}^p = \left\{ A \in \mathcal{K}(\mathcal{H}) : \|A\|_p := \left(\sum_{k=1}^{\infty} s_k^p(A) \right)^{\frac{1}{p}} < \infty \right\}, \quad p \in [1, \infty),$$

where $s_k(A)$ are the singular numbers of A (i.e., the eigenvalues of $|A| = \sqrt{A^*A}$). The norm $\|A\|_p := \left(\sum_{k=1}^{\infty} s_k^p(A) \right)^{\frac{1}{p}}$ is called the Schatten p -norm of A .

Note that \mathcal{S}^1 and \mathcal{S}^2 in the above definition are called the trace class and the Hilbert-Schmidt class of operators, respectively.

Definition 4.1.4. [17, Chapter VI, Section 6] The map $\text{Tr} : \mathcal{S}^1 \mapsto \mathbb{C}$ given by

$$\text{Tr}(A) = \sum_{n=1}^{\infty} \langle A\phi_n, \phi_n \rangle,$$

where $\{\phi_n\}$ is any orthonormal basis, is called the trace of A and it is independent of the choice of the basis $\{\phi_n\}$.

4.2 Convergence of a Sequence of Operators

Definition 4.2.1. [12, Definition 4.9-1] Let X and Y be normed spaces. A sequence $\{T_n\}$ of operators $T_n \in \mathcal{B}(X, Y)$ is said to be convergent to $T \in \mathcal{B}(X, Y)$

(1) in the uniform operator topology if

$$\|T_n - T\| \rightarrow 0, \quad \text{as } n \rightarrow \infty;$$

(2) in the strong operator topology if

$$\|T_n x - T x\| \rightarrow 0, \quad \text{as } n \rightarrow \infty \quad \text{for all } x \in X;$$

(3) in the weak operator topology if

$$|f(T_n x) - f(T x)| \rightarrow 0, \quad \text{as } n \rightarrow \infty \quad \text{for all } x \in X \text{ and for all } f \in Y'.$$

4.3 Spectral Measure and Spectral Integral

The material in this section is standard and found in many books in Functional Analysis. We refer the reader to chapters 5 and 6 of [4] for more details.

4.3.1 Spectral Measure

Definition 4.3.1. [4, Chapter 5, Section 1] Let (Ω, Σ) be a measurable space and $\mathcal{P} = \mathcal{P}(\mathcal{H})$ be the set of all orthogonal projections on \mathcal{H} . Then, a spectral measure E on (Ω, Σ) with respect to \mathcal{H} is a mapping $E : \Sigma \mapsto \mathcal{P}$ satisfying the following two conditions.

(1) E is countably additive, that is for any sequence $\{\delta_n\}_{n=1}^{\infty}$ of pairwise disjoint sets from Σ , we have $E(\bigcup_{n=1}^{\infty} \delta_n) = \sum_{n=1}^{\infty} E(\delta_n)$, where the latter series converges in the strong operator topology.

(2) $E(\Omega) = I$, where I is the identity on \mathcal{H} .

Using the additivity of E , one can prove the following additional properties.

Theorem 4.3.2. [4, Theorems 5.1.1 and 5.1.2] *Let E be a spectral measure on (Ω, Σ) with respect to \mathcal{H} and let $\{\delta_n\}_{n \in \mathbb{N}}$ be measurable subsets of Ω .*

(1) *For $\delta_1, \delta_2 \in \Sigma$, we have*

$$E(\delta_1)E(\delta_2) = E(\delta_2)E(\delta_1) = E(\delta_1 \cap \delta_2).$$

In particular, $E(\delta_1)E(\delta_2) = 0$ if $\delta_1 \cap \delta_2 = \emptyset$.

(2) *If $\delta_n \subset \delta_{n+1}$ for all $n \in \mathbb{N}$, then*

$$\lim_{n \rightarrow \infty} E(\delta_n) = E\left(\bigcup_{n=1}^{\infty} \delta_n\right),$$

where the limit is evaluated in the strong operator topology.

(3) *If $\delta_{n+1} \subset \delta_n$ for all $n \in \mathbb{N}$, then*

$$\lim_{n \rightarrow \infty} E(\delta_n) = E\left(\bigcap_{n=1}^{\infty} \delta_n\right),$$

where the limit is evaluated in the strong operator topology.

Note that every spectral measure E generates a family of finite scalar measures $\langle E(\delta)\xi, \eta \rangle$, $\xi, \eta \in \mathcal{H}$ and $\delta \in \Sigma$.

4.3.2 Spectral Integral of Bounded Measurable Functions

Definition 4.3.3. [4, Chapter 5, Section 3] *Let $(\Omega, \Sigma, \mathcal{H}, E)$ be a spectral measure space and let $S(\Omega, E)$ denote the set of all simple functions on Ω . Then the integral of $f \in S(\Omega, E)$ with respect to E is the operator T_f^E defined by*

$$T_f^E = \int_{\Omega} f(\omega) dE(\omega) := \sum_{k=1}^n \alpha_k E(\delta_k), \quad (4.3.1)$$

where $f \in S(\Omega, E)$ is of the form

$$f = \sum_{k=1}^n \alpha_k \chi_{\delta_k}, \quad \alpha_k \in \mathbb{C}, \quad \delta_k \in \Sigma, \quad k = 1, \dots, n, \quad \bigcup_{k=1}^n \delta_k = \Omega, \quad n \in \mathbb{N},$$

and χ_{δ} is a characteristic function of the set $\delta \in \Sigma$.

The spectral integral defined by the equation (4.3.1) satisfies the following properties.

Theorem 4.3.4. [4, Chapter 5, Section 3] Let T_f^E be as in (4.3.1), $f, g \in S(\Omega, E)$, T_f a shorthand of T_f^E , \bar{f} a complex conjugate of f , and I the identity on \mathcal{H} . Then

- (1) $T_{\alpha f + \beta g} = \alpha T_f + \beta T_g$, $\alpha, \beta \in \mathbb{C}$;
- (2) $T_{fg} = T_f T_g = T_g T_f$;
- (3) $(T_f)^* = T_{\bar{f}}$;
- (4) $T_f = I$, for $f \equiv 1$;
- (5) $\langle T_f \xi, \eta \rangle = \int_{\Omega} f(\lambda) d \langle E(\lambda) \xi, \eta \rangle$, $\xi, \eta \in \mathcal{H}$;
- (6) $\|T_f \xi\|_{\mathcal{H}}^2 = \int_{\Omega} |f(\lambda)|^2 d \langle E(\lambda) \xi, \xi \rangle$;
- (7) $\|T_f\| = \|f\|_{\infty}$,

where $\|\cdot\|_{\mathcal{H}}$ and $\|\cdot\|$ denote respectively the norm on \mathcal{H} and the operator norm on $\mathcal{B}(\mathcal{H})$.

Definition 4.3.5. [4, Chapter 5, Section 3] Let $(\Omega, \Sigma, \mathcal{H}, E)$ be a spectral measure space. Then, the integral of a bounded measurable function f on Ω with respect to E is defined by

$$T_f := \int_{\Omega} f(\omega) dE(\omega) = \lim_{n \rightarrow \infty} \int_{\Omega} f_n(\omega) dE(\omega), \quad (4.3.2)$$

where the limit is evaluated in the operator norm on $\mathcal{B}(\mathcal{H})$, and $\{f_n\}_{n \in \mathbb{N}}$ is an arbitrary sequence of simple functions converging uniformly to f .

Theorem 4.3.6. [4, Chapter 5, Section 3] Let T_f be as in (4.3.2), f, g bounded measurable functions on Ω , \bar{f} a complex conjugate of f , and I the identity on \mathcal{H} . Then

- (1) $T_{\alpha f + \beta g} = \alpha T_f + \beta T_g$, $\alpha, \beta \in \mathbb{C}$;
- (2) $T_{fg} = T_f T_g = T_g T_f$;
- (3) $(T_f)^* = T_{\bar{f}}$;
- (4) $T_f = I$, for $f \equiv 1$;
- (5) $\langle T_f \xi, \eta \rangle = \int_{\Omega} f(\lambda) d \langle E(\lambda) \xi, \eta \rangle$, $\xi, \eta \in \mathcal{H}$;
- (6) $\|T_f \xi\|_{\mathcal{H}}^2 = \int_{\Omega} |f(\lambda)|^2 d \langle E(\lambda) \xi, \xi \rangle$;
- (7) $\|T_f\| = \|f\|_{\infty}$,

where $\|\cdot\|_{\mathcal{H}}$ and $\|\cdot\|$ denote respectively the norm on \mathcal{H} and the operator norm on $\mathcal{B}(\mathcal{H})$.

4.3.3 Spectral Theorem for Bounded Self-adjoint Operators

Theorem 4.3.7. [17, Theorem VII.8] Let H_0 be a bounded self-adjoint operator on \mathcal{H} . Let $[a, b] \subset \mathbb{R}$ such that $\sigma(H_0) \subset [a, b]$. Then there exists a unique spectral measure

$E := E_{H_0}$ on the Borel σ -algebra $\mathfrak{B}([a, b])$ such that

$$H_0 = \int_{[a, b]} \lambda dE(\lambda),$$

where the convergence of the integral is understood in the uniform operator topology.

4.3.4 Spectral Theorem for Unbounded Self-adjoint Operators

Theorem 4.3.8. [17, Theorem VIII.6] *Let H_0 be a self-adjoint operator in \mathcal{H} . Then there exists a unique spectral measure $E := E_{H_0}$ on the Borel σ -algebra $\mathfrak{B}(\mathbb{R})$ such that*

$$H_0 = \int_{\mathbb{R}} \lambda dE(\lambda),$$

where the convergence of the integral is understood in the strong operator topology.

4.3.5 Functional Calculus

Let f be a bounded measurable function on Ω and let us write $f(H_0)$ for the spectral integral T_f of Definition 4.3.5. Then, we have

$$f(H_0) = \int_{\mathbb{R}} f(\lambda) dE(\lambda).$$

The assignment $f \rightarrow f(H_0)$ is called the functional calculus of the self-adjoint operator H_0 .

4.4 Bochner Integrals

The Bochner integral is the natural generalization of the Lebesgue integral to functions that take values in a Banach space. In this section, we give a definition of the Bochner integral and state a version of the dominated convergence theorem for it. For more details about the topic, we refer the reader to [19].

Definition 4.4.1. [19, Definition 4.1] *A function f defined on a measure space (X, Σ, μ) with values in a Banach space \mathbf{B} is said to be weakly measurable if for any $\alpha \in X^*$, the numerical function $\alpha(f(x))$ of x is measurable. $f(x)$ is said to be measurable if there exists a sequence of simple functions with values in a Banach space \mathbf{B} convergent to $f(x)$ μ -a.e. on X .*

Recall that a simple function with values in a Banach space \mathbf{B} is a function of the form

$$f = \sum_{n=1}^N b_n \chi_{\delta_n}, \quad N \in \mathbb{N},$$

where $b_n \in \mathbf{B}$ and the sets $\delta_n \in \Sigma$ are disjoint.

Definition 4.4.2. [19, Definition 4.2] A function f defined on a measure space (X, Σ, μ) with values in a Banach space \mathbf{B} is said to be separably-valued if its range $\{f(x) : x \in X\}$ is separable. It is μ -almost separably-valued if there exists a measurable set B of μ -measure zero such that $\{f(x) : x \in X \setminus B\}$ is separable.

Theorem 4.4.3. (B. J. Pettis)[19, Theorem 4.3] A function f defined on a measure space (X, Σ, μ) with values in a Banach space \mathbf{B} is measurable if and only if it is weakly measurable and μ -almost separably-valued.

Definition 4.4.4. [19, Chapter V, Section 5] A function f defined on a measure space (X, Σ, μ) with values in a Banach space \mathbf{B} is said to be Bochner μ -integrable if there exists a sequence of simple functions $\{f_n\}_{n \geq 1}$ which converges to f μ -a.e. in such a way that

$$\lim_{n \rightarrow \infty} \int_X \|f_n - f\|_{\mathbf{B}} d\mu = 0.$$

In this case, the Bochner μ -integral of f is defined by

$$\int_X f d\mu = \lim_{n \rightarrow \infty} \int_X f_n d\mu.$$

Theorem 4.4.5. (S. Bochner)[19, Theorem 5.1] Let (X, Σ, μ) be a measure space. A measurable function f with values in a Banach space \mathbf{B} is Bochner μ -integrable if and only if $\|f(x)\|_{\mathbf{B}}$ is μ -integrable.

Proposition 4.4.6. (Dominated convergence theorem) Let $f_n : X \mapsto \mathbf{B}$ be a sequence of functions, each of which is Bochner μ -integrable. Assume that there exist a function $f : X \mapsto \mathbf{B}$ and a μ -integrable function $g : X \mapsto \mathbb{C}$ such that

- (1) $\lim_{n \rightarrow \infty} f_n = f$ μ -almost everywhere;
- (2) $\|f_n\|_{\mathbf{B}} \leq |g|$ μ -almost everywhere.

Then, f is Bochner μ -integrable and we have

$$\lim_{n \rightarrow \infty} \int_X \|f_n - f\|_{\mathbf{B}} d\mu = 0.$$

In particular we have

$$\lim_{n \rightarrow \infty} \int_X f_n d\mu = \int_X f d\mu.$$

4.5 The Schwartz class and the Fourier Transform

The material discussed in this section is standard and found in many books in Fourier Analysis. We refer the reader to [9] and [15] for more details.

4.5.1 The Class of Schwartz Functions

Definition 4.5.1. [9, Definition 2.2.1] A C^∞ complex-valued function f on \mathbb{R} is called a Schwartz function if for every integers $k, l \geq 0$ there exists a constant $M_{k,l} > 0$ such that

$$\sup_{x \in \mathbb{R}} |x|^k |f^{(l)}(x)| \leq M_{k,l}.$$

The set of all Schwartz functions on \mathbb{R} is denoted by $\mathcal{S}(\mathbb{R})$.

4.5.2 The Fourier Transform

Definition 4.5.2. [9, Chapter 2.2.4] Let $f \in L^1(\mathbb{R})$. Then the Fourier transform of f denoted by \hat{f} is given by

$$\hat{f}(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(\lambda) e^{-i\lambda t} d\lambda.$$

Proposition 4.5.3. (Riemann-Lebesgue Lemma)[15, Lemma 8.5.1] For a function $f \in L^1(\mathbb{R})$ we have that

$$|\hat{f}(t)| \rightarrow 0 \quad \text{as } |t| \rightarrow \infty.$$

Proposition 4.5.4. [9, Exercise 2.2.6] If $f \in L^1(\mathbb{R})$, then \hat{f} is uniformly continuous on \mathbb{R} .

Definition 4.5.5. [9, Chapter 2.2.4] Let $g \in L^1(\mathbb{R})$. Then the inverse Fourier transform of g denoted by $(g)^\vee$ is given by

$$(g)^\vee(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} g(t) e^{i\lambda t} dt.$$

Note that if both $f, \hat{f} \in L^1(\mathbb{R})$, then we have $(\hat{f})^\vee = f$ a.e.

Proposition 4.5.6. (See [15, Chapter 7, Section 3]) If f is such that $f^{(j)}, \widehat{f^{(j)}} \in L^1(\mathbb{R})$, $j = 0, 1, \dots, n$, then

$$\widehat{f^{(j)}}(\lambda) = (i\lambda)^j \hat{f}(\lambda), \quad j = 0, 1, \dots, n.$$

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