Trace Formulas and Finite Dimensional Approximations

by

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to the

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Declaration

I hereby declare that the work contained in the thesis entitled **"Trace Formulas and Finite Dimensional Approximations"** has been done by me, a student in the Department of Mathematics, Indian Institute of Technology Guwahati, under the guidance of **Dr. Arup Chattopadhyay**, Indian Institute of Technology Guwahati, for the award of **Doctor of Philosophy** and that this work has not been submitted elsewhere for a degree.

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Certificate

It is certified that the work contained in the thesis titled **"Trace Formulas and Finite Dimensional Approximations"** by **Chandan Pradhan (186123006)**, a student in the Department of Mathematics, Indian Institute of Technology Guwahati, for the award of the degree of **Doctor of Philosophy** has been carried out under my supervision and this work has not been submitted elsewhere for a degree.

Guwahati
April, 2023

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Dedicated

To

My Grandfather
Late Barendranath Pradhan (Dadu)

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Chandan Pradhan

Abstract

The dissertation gives a new proof of some existing second-order trace formulas, namely the Koplienko-Neidhardt trace formula for pair of unitaries in the multiplicative path, the Koplienko-Neidhardt trace formula for pair of contractions via linear path with one of them being normal. Our proofs are based on the idea of the finite-dimensional approximation method introduced by Voiculescu. As a consequence of our results and the Schäffer matrix unitary dilation, we obtained second-order trace formula for a class of pairs of contractions via linear path. Using a different setup of finite dimensional approximations, we extend the Koplienko-Neidhardt trace formula for a class of pairs of contractions via multiplicative path.

Moreover, in this thesis, using the dilation theory and the existing higher-order trace formula for pair of unitaries via multiplicative path, we obtain a higher-order trace formulae for a class of pairs of contractions and a class of pairs of maximal dissipative operators via multiplicative path.

Finally, this dissertation establishes estimates and an integral representation for the higher order Taylor remainder of the spectral action functional $V \mapsto \mathrm{Tr}(f(H_0 + V))$ on bounded self-adjoint perturbations, where H_0 is a self-adjoint operator with compact resolvent and f belongs to a 'nice' class of scalar functions.

Introduction

Koplienko [31] found a trace formula for perturbations of self-adjoint operators by operators of Hilbert-Schmidt class $\mathcal{B}_2(\mathcal{H})$. Later in 1988, a similar formula was obtained by Neidhardt [42] in the case of unitary operators. In this dissertation, we give a still another proof of the Koplienko-Neidhardt trace formula in the case of unitary operators by reducing the problem to a finite-dimensional one as in the proof of Krein's trace formula by Voiculescu [75], Sinha and Mohapatra [63, 41]. Chapter 2 is devoted to the above-mentioned new proof.

In 2012, Potapov and Sukochev [56] obtained a trace formula like the Koplienko trace formula for pairs of contractions by answering an open question posed by Gesztesy, Pushnitski, and Simon in [26, Open Question 11.2]. In Chapter 3, we supply a new proof of the Koplienko trace formula in the case of pair of contractions (T, T_0), where the initial operator T_0 is normal, via linear path by reducing the problem to a finite-dimensional one as in the proof of Krein's trace formula by Voiculescu [75], Sinha and Mohapatra [63, 41]. Consequently, we obtain the Koplienko trace formula for a class of pairs of contractions using the Schäffer matrix unitary dilation. Moreover, we also obtain the Koplienko trace formula for a pair of self-adjoint operators and maximal dissipative operators using the Cayley transform. At the end, we extend the Koplienko-Neidhardt trace formula for a class of pair of contractions (T, T_0) via multiplicative path using finite-dimensional approximation method.

In [40], Marcantognini and Morán obtained Koplienko-Neidhardt trace formula for pairs of contractions and pairs of maximal dissipative operators via multiplicative path. In Chapter 4 of this dissertation, we prove the existence of higher-order spectral shift functions for pairs of contractions and pairs of maximal dissipative operators via multiplicative path by adapting the argument employed in [40].

Finally, in Chapter 5, we establish estimates and representations for the remainders of Taylor approximations of the spectral action functional $V \mapsto \mathrm{Tr}(f(H_0 + V))$ on bounded self-adjoint perturbations, where H_0 is a self-adjoint operator with compact resolvent on a complex separable Hilbert space and f belongs to a broad set of compactly supported functions including n-times differentiable function with bounded n-th derivative. Our results significantly extend analogous results in [67], where f was assumed to be compactly supported and $(n+1)$-times continuously differentiable. If, in addition, the resolvent of H_0 belongs to Schatten p-class, stronger estimates are derived and extended to noncompactly supported functions with suitable decay at infinity.

Papers

This thesis is based on four papers.

1) Chapter 2 based on [18] (joint with Arup Chattopadhyay and Soma Das, and published in J. Math. Anal. Appl.)

2) Chapter 3 based on [17] (joint with Arup Chattopadhyay and Soma Das, and available in arXiv).

3) Chapter 4 based on [19] (joint with Arup Chattopadhyay and published in New York Journal of Mathematics).

4) Chapter 5 based on [20] (joint with Arup Chattopadhyay and Anna Skripka, and available in arXiv).

Abbreviation and Notation

$\mathbb{N}$	The set of all natural numbers
$\mathbb{Z}$	The set of all integers
$\mathbb{R}$	The set of all real numbers
$\mathcal{H}$	Complex separable Hilbert space
$\mathcal{B}(\mathcal{H})$	Algebra of bounded linear operators on $\mathcal{H}$
$\mathcal{B}_f(\mathcal{H})$	Space of all finite rank operators on $\mathcal{H}$
$\mathcal{B}_0(\mathcal{H})$	Space of all compact operators on $\mathcal{H}$
$\mathcal{B}_1(\mathcal{H})$	Space of trace class operators on $\mathcal{H}$
$\mathcal{B}_2(\mathcal{H})$	Space of Hilbert-Schmidt operators on $\mathcal{H}$
$\mathcal{B}_n(\mathcal{H})$	Schatten n-class operators on $\mathcal{H}$
$E_H(\cdot)$	Spectral measure of the self-adjoint operator H
$\mathcal{E}_T(\cdot)$	Semi-spectral measure of the contraction T
Tr	The trace
$\|T\|$	Positive square root of T^*T
Dom(T)	Domain of T

Contents

CHAPTER 1

Preliminaries

In this chapter we recall some fundamental results in operator theory.

1.1 Algebra of bounded operators

Definition 1.1.1. *An inner product space* $(\mathcal{H}, \langle\cdot,\cdot\rangle_{\mathcal{H}})$ *over a field* $\mathbb{F}$ *is said to be a Hilbert space if it is a Banach space with respect to the norm induced by the inner product* $\langle\cdot,\cdot\rangle_{\mathcal{H}}$*. A Hilbert space is said be a complex (real) Hilbert space if* $\mathbb{F} = \mathbb{C}$ *(*$\mathbb{F} = \mathbb{R}$*).*

Throughout the thesis, $\mathcal{H}$ is a complex separable Hilbert space. We denote $\mathcal{B}(\mathcal{H})$ by the space of all bounded linear operators on $\mathcal{H}$. It is well known that $\mathcal{B}(\mathcal{H})$ is a non-commutative C^*-algebra.

1.1.1 The Trace

Definition 1.1.2. *Let* T *be a positive bounded linear operator on* $\mathcal{H}$*, choose an orthonormal basis* $\{e_i\}_{i=1}^{\infty}$ *for* $\mathcal{H}$*. Then the trace of* T *is denoted by* $\mathrm{Tr}(T)$ *and is defined by*

$$\mathrm{Tr}(T) = \sum_{i=1}^{\infty} \langle Te_i, e_i\rangle, \tag{1.1}$$

with values in $[0, \infty]$.

Remark 1.1.3. *From the above Definition* (1.1.2)*, it follows that* $\operatorname{Tr}(T^*T) = \operatorname{Tr}(TT^*)$*, which further follows that* Tr *is independent of the choice of orthonormal basis (see, e.g., [46, Proposition 3.4.3, and Corollary 3.4.4]).*

For a bounded operator $T \in \mathcal{B}(\mathcal{H})$, $|T|$ denotes the unique positive square root of T^*T and we write $|T| = (T^*T)^{\frac{1}{2}}$. For $p > 0$, we denote the space of Schatten p-class operators by $\mathcal{B}_p(\mathcal{H})$ and is defined as follows

$$\mathcal{B}_p(\mathcal{H}) := \{T \in \mathcal{B}(\mathcal{H}) : \|T\|_p = \big(\operatorname{Tr}(|T|^p)^{\frac{1}{p}}\big) < \infty\}.$$

For $p = 1$, the collection $\mathcal{B}_1(\mathcal{H})$ is called the space of trace class operators and for $p = 2$, the collection $\mathcal{B}_2(\mathcal{H})$ is called Hilbert-Schmidt space and the operators in $\mathcal{B}_2(\mathcal{H})$ are called the Hilbert-Schmidt operators. Since, any bounded operator can be written as the linear combination of four positive bounded operators, therefore the Definition 1.1.2 of trace can be extended for a trace class operator T, where the series (1.1) converges absolutely. Moreover, as in the case of positive operators, for trace class operators, the Tr is also independent of the choice of orthonormal basis. The subspace relation between these Schatten p-classes is given by the following result.

Proposition 1.1.4. *The classes* $\mathcal{B}_p(\mathcal{H})$*,* $1 \le p < \infty$*, are the self-adjoint ideals in* $\mathcal{B}(\mathcal{H})$ *and*

$$\mathcal{B}_f(\mathcal{H}) \subset \mathcal{B}_1(\mathcal{H}) \subset \mathcal{B}_2(\mathcal{H}) \subset \cdots \subset \mathcal{B}_0(\mathcal{H}) \subset \mathcal{B}(\mathcal{H}),$$

where $\mathcal{B}_f(\mathcal{H})$ *and* $\mathcal{B}_0(\mathcal{H})$ *are the space of all finite rank operators and compact operators on* $\mathcal{H}$ *respectively.*

Theorem 1.1.5. *The ideal* $\mathcal{B}_2(\mathcal{H})$ *form a Hilbert space under the inner product*

$$\langle S, T\rangle = \operatorname{Tr}(T^*S), \quad S, T \in \mathcal{B}_2(\mathcal{H}).$$

The Hilbert-Schmidt space is separable when $\mathcal{H}$ is separable and the orthonormal basis of $\mathcal{B}_2(\mathcal{H})$ is given by the following proposition.

Proposition 1.1.6. *Let* $\{e_i\}_{i\in\mathbb{N}}$ *be an orthonormal basis for* $\mathcal{H}$*, then the collection*

$$\Big\{e_i \odot e_j : i, j \in \mathbb{N}\Big\}$$

of rank one operators form an orthonormal basis for $\mathcal{B}_2(\mathcal{H})$*, where* $e_i \odot e_j$ *is a rank one operator defined by* $e_i \odot e_j(h) = \langle h, e_j\rangle e_i$ *for all* $h \in \mathcal{H}$*.*

The following well-known inequalities shows that the Schatten p-class $\mathcal{B}_p(\mathcal{H})$ forms an ideal in $\mathcal{B}(\mathcal{H})$.

Lemma 1.1.7. *Let $p > 0$, $S \in \mathcal{B}(\mathcal{H})$ and $T \in \mathcal{B}_p(\mathcal{H})$, then $\|ST\|_p \leq \|S\|\|T\|_p$.*

Theorem 1.1.8. *[27, Page 92] (**Hölder-von Neumann inequality**): Let $1 < r \leq p \leq 2 \leq q < \infty$, such that $p^{-1} + q^{-1} = r^{-1}$. Let $S \in \mathcal{B}_p(\mathcal{H})$, $T \in \mathcal{B}_q(\mathcal{H})$. Then $ST \in \mathcal{B}_r(\mathcal{H})$ and*

$$\|ST\|_r \leq \|S\|_p \|T\|_q, \quad S \in \mathcal{B}_p(\mathcal{H}), T \in \mathcal{B}_q(\mathcal{H}).$$

1.2 Spectral Theorem

Definition 1.2.1. *(Partial Isometry) A partial isometry W on a separable Hilbert space $\mathcal{H}$ is a bounded linear operator on $\mathcal{H}$ such that for each h in $(\ker W)^{\perp}$, $\|Wh\| = \|h\|$. The space $(kerW)^{\perp}$ is called the initial space of W and the range space $R(W)$ is called the final space of W.*

Now we give the spectral properties of a unitary operator on $\mathcal{H}$, after that, we show that how a densely defined self-adjoint operator can be transformed to a unitary operator.

Definition 1.2.2. *(Unitary Operator) A unitary operator U on $\mathcal{H}$ is a bounded linear operator, which satisfied $UU^* = U^*U = I$. So a unitary operator on $\mathcal{H}$ is also an isometry on $\mathcal{H}$. The adjoint of a unitary operator is its inverse.*

Remark 1.2.3. *Suppose A is a partial isometry on $\mathcal{H}$, then A is unitary if it is bijective.*

Proof. Let A be a partial isometry on $\mathcal{H}$ with $kerA = \{0\}$, then its initial space is the full space $\mathcal{H}$ and $\|Ah\| = \|h\|, \quad \forall h \in \mathcal{H}$. This shows that A is an unitary operator on $\mathcal{H}$. □

Lemma 1.2.4. *If U is a unitary operator on $\mathcal{H} \neq 0$, then the spectrum of U, $\sigma(U)$ is a closed subset of the unit circle, that is for $\lambda \in \sigma(U)$, $|\lambda| = 1$.*

1.2.1 Unbounded Operators

In this section, we introduce some basic facts of unbounded operators, the spectral theorem for self-adjoint operators and unitary operators.

1.2.2 Basic Definitions

Definition 1.2.5. ***(Domain)***: *Let $\mathcal{H}$ and $\mathcal{K}$ be two Hilbert spaces and let A be a linear operator from $\mathcal{H}$ to $\mathcal{K}$, then the domain of the operator A is the linear subspace of $\mathcal{H}$, where the operator is well defined. We denote the domain of A by* $\mathrm{Dom}(A)$.

Definition 1.2.6. ***(Densely Defined operators)*** *A linear operator $A : \mathcal{H} \to \mathcal{K}$ with domain* $\mathrm{Dom}(A)$ *is called densely defined operator if $cl[\mathrm{Dom}(A)] = \mathcal{H}$, where $cl[\mathrm{Dom}(A)]$ is the closure of* $\mathrm{Dom}(A)$.

Definition 1.2.7 (Closed operator and Closable operator). *A linear operator $A : \mathcal{H} \to \mathcal{K}$ is said to be a closed operator if its graph is closed in $\mathcal{H} \times \mathcal{K}$. An operator is said to be closable if it has a closed extension. We use the notation $\mathcal{C}(\mathcal{H}, \mathcal{K})$ for the collection of all closed densely defined operators from $\mathcal{H}$ into $\mathcal{K}$.*

Definition 1.2.8 (Adjoint operator). *Let $A : H \to K$ be a densely defined operator, then the adjoint of A is denote by $A^* : \mathcal{K} \to \mathcal{H}$ and its domain is defined by* $\mathrm{Dom}(A^*) = \{k \in \mathcal{K} : h \longmapsto \langle Ah, k\rangle$ *is a bounded linear functional on* $\mathrm{Dom}(A)\}$.

Definition 1.2.9 (Self-adjoint operator). *Let $A : \mathcal{H} \to \mathcal{H}$ be a closed densely defined operator. Then A is called a self-adjoint operator if $A = A^*$.*

Definition 1.2.10 (Dissipative operator). *Let $A : \mathcal{H} \to \mathcal{H}$ be a linear operator (need not be bounded) with dense domain* $\mathrm{Dom}(A)$ *called dissipative if* $\mathrm{Im}\langle Ah, h\rangle \geq 0$ *for all* $h \in \mathrm{Dom}(A)$. *A dissipative operator is called maximal if it has no proper dissipative extension.*

1.2.3 The Cayley Transform

The following lemma deals with the fact that given a unitary operator U_0, by suitably rotating the spectrum of U_0, or equivalently defining a new unitary operator $U_0' = e^{-i\phi}U_0$ we get a self-adjoint operator H_0 such that U_0' is the Cayley transform of H_0, that is $U_0' = (i - H_0)(i + H_0)^{-1}$. Note that the proof of this lemma is available in [41, Theorem 1.1] but for reader's convenience we are providing a proof herewith.

Lemma 1.2.11. *Let U_0 be an unitary operator in a separable Hilbert space $\mathcal{H}$. Then there exists $\phi \in (-\pi, \pi]$ such that $\left(e^{i\phi} + U_0\right)$ is one to one, and hence invertible. Furthermore, the* *operator*

$$\begin{aligned} H_0 &= -i\left(-e^{i\phi}+U_0\right)\left(e^{i\phi}+U_0\right)^{-1} \\ &= i\left(I-e^{-i\phi}U_0\right)\left(I+e^{-i\phi}U_0\right)^{-1} \\ &\equiv i\left(I-U_0^{'}\right)\left(I+U_0^{'}\right)^{-1} \end{aligned} \tag{1.2}$$

is self-adjoint.

Proof. Since $\mathcal{H}$ is separable, then the eigenvalues of U_0 are at most countable. Therefore there exists some $\phi \in (-\pi, \pi]$ such that $-e^{i\phi} \notin \sigma_p(U_0)$ (set of eigenvalues of U_0) and hence $\left(I+U_0^{'}\right)$ is invertible, where $U_0^{'} = e^{-i\phi}U_0$. Note that the following identity

$$\text{Ran}\left(I+U_0^{'}\right)^{\perp} = \text{Ker}\left(I+U_0^{'*}\right) = \text{Ker}\left(I+U_0^{'}\right) = \{0\}$$

implies that the operator H_0 in (1.2) is densely defined and furthermore H_0 is also symmetric in this domain. Next we also observe that the ranges of $i+H_0 = 2i\left(I+U_0^{'}\right)^{-1}$ and of $i-H_0 = 2iU_0^{'}\left(I+U_0^{'}\right)^{-1}$ are the whole Hilbert space since $\text{Ran}\left\{\left(I+U_0^{'}\right)^{-1}\right\} = \text{Dom}\left(I+U_0^{'}\right) = \mathcal{H}$ and $U_0^{'}$ is unitary. Thus H_0 is self-adjoint and hence the proof. ☐

Next we state the Cayley transformation of maximal dissipative operators as follows:

Lemma 1.2.12. *[70, Theorem 4.1] The Cayley transform of a maximal dissipative operator A is a contraction $T : \mathcal{H} \to \mathcal{H}$ given by $T = (i-A)(i+A)^{-1}$ such that $\ker T = \ker(i-A)$ and $\ker T^* = \ker(A^*+i)$. Moreover, a contraction T is the Cayley transform of a maximal dissipative operator A if and only if -1 is not an eigenvalue of T*

Next, we give the spectral theorem for self-adjoint operators and unitary operators.

1.2.4 The Spectral Theorem

Definition 1.2.13. *A family $\{E_\lambda\}_{\lambda\in\mathbb{R}}$ of orthogonal projection in $\mathcal{B}(\mathcal{H})$ is said to be spectral family if they satisfy following conditions:*

(i) $\{E_\lambda\}_{\lambda\in\mathbb{R}}$ *is non-decreasing, that is* $E_\lambda \le E_\mu$ *for* $\lambda \le \mu$, *equivalently* $E_\lambda E\mu = E_{\min\{\lambda,\mu\}}$,

(ii) $SOT-\lim\limits_{\lambda\to-\infty} E_\lambda = 0$ *and* $SOT-\lim\limits_{\lambda\to\infty} E_\lambda = I$,

(iii) $SOT-\lim_{\eta\to 0^+} E_{\lambda+\eta} = E_\lambda$,

where $SOT-\lim$ *is the limit in the strong operator topology.*

Next we state the spectral theorem of self-adjoint operator in $\mathcal{H}$.

Theorem 1.2.14. *[4, Proposition 5.8] Let* H *be a self-adjoint operator in* $\mathcal{H}$*. Then there is a unique spectral family* $\{E_\lambda\}_{\lambda\in\mathbb{R}}$ *such that*

(i) $H = \int_{\mathbb{R}} \lambda E(d\lambda)$;

(ii) if $A \in \mathcal{B}(\mathcal{H})$ *such that* $AH \subseteq HA$*, then* $A\big(\int_{\mathbb{R}} \phi(\lambda)E(d\lambda)\big) = \big(\int_{\mathbb{R}} \phi(\lambda)E(d\lambda)\big)A$*, for every bounded continuous function* ϕ *on* $\mathbb{R}$.

The following theorem state the spectral theorem for unitary.

Theorem 1.2.15. *[57, Page 281] Let* U *be a unitary operator on* $\mathcal{H}$*. Then there is a spectral family* $\{E_t\}_{t\in[0,2\pi]}$ *on the line segment* $0 \le t \le 2\pi$*, such that*

(i) $U = \int_0^{2\pi} e^{it}E(dt)$;

(ii) if $A \in \mathcal{B}(\mathcal{H})$ *such that* $AU = UA$*, then* $A\big(\int_0^{2\pi} \phi(t)E(dt)\big) = \big(\int_0^{2\pi} \phi(t)E(dt)\big)A$*, for every continuous function* ϕ *on* $\mathbb{R}$.

We can require that E_t *be continuous at the point* $t = 0$*, that is* $E_0 = 0$*;* $\{E_t\}_{t\in[0,2\pi]}$ *will then be determined uniquely by* U.

1.3 Double operator integrals

Let $E_1(\cdot)$ and $E_2(\cdot)$ be two spectral measures given on Borel σ-algebra $\mathfrak{B}(\mathbb{R})$, with values in the set of orthogonal projections in $\mathcal{B}(\mathcal{H})$. Let us consider

$$\mathcal{E}_1(\delta) : X \mapsto E_1(\delta)X, \quad \mathcal{E}_2(\delta) : X \mapsto XE_2(\Delta), \text{ where } \delta, \Delta \in \mathfrak{B}(\mathbb{R}), X \in \mathcal{B}_2(\mathcal{H}). \tag{1.3}$$

It is clear that $\mathcal{E}_1(\cdot)$ and $\mathcal{E}_2(\cdot)$ are commuting spectral measures on $\mathfrak{B}(\mathbb{R})$ with respect to $\mathcal{B}_2(\mathcal{H})$. Now we define the product of the measures $\mathcal{E}_1(\cdot)$ and $\mathcal{E}_2(\cdot)$ by

$$G(\delta\times\Delta) := \mathcal{E}_1(\delta)\times\mathcal{E}_2(\Delta), \quad \delta, \Delta \in \mathfrak{B}(\mathbb{R}), \text{ so that } G(\delta\times\Delta)(X) = \mathcal{E}_1(\delta)\, X\, \mathcal{E}_2(\Delta), X \in \mathcal{B}_2(\mathcal{H}). \tag{1.4}$$

By [69, Proposition 2.5.1] (see also [9, Theorem 2]), we conclude that the above measure $G(\cdot)$ is a spectral measure on $(\mathbb{R}^2, \mathfrak{B}(\mathbb{R}^2))$ with respect to $\mathcal{B}_2(\mathcal{H})$, where $\mathfrak{B}(\mathbb{R}^2)$ is the Borel σ-algebra on $\mathbb{R}^2$.

Definition 1.3.1. *Assume above notations. Let Φ be a continuous bounded function on $\mathbb{R}^2$. The Birman–Solomyak double operator integral is defined as the integral of the symbol Φ with respect to the spectral measure G, that is,*

$$T_{\Phi}^{G}(X) := \int_{\mathbb{R}^2} \Phi(\lambda_1, \lambda_2)\, dG(\lambda_1, \lambda_2)(X) \tag{1.5}$$

The above operator integral $T_{\Phi}^{G}(X)$ is understood in Stieltjes' sense. Moreover, T_{Φ}^{G} is bounded on $\mathcal{B}_2(\mathcal{H})$ and $\|T_{\Phi}^{G}\| = \|\Phi\|_{\infty}$. For more on the theory of double operator integral, we refer [12, 10, 11, 69].

1.4 Bochner Integral

The Bochner integral is the natural generalization of the familiar Lebesgue integral to the vector-valued setting. Here we only state some useful results related to the Bochner integration, for more details, we refer [28, Chapter 1]. Throughout this section, $(\Omega, \mathscr{A}, \mu)$ is a σ-finite measure space and $\mathcal{X}$ is a Banach space. A μ-simple function $f : \Omega \to \mathcal{X}$ is of the form $\sum_{k=1}^{n} x_k 1_{A_k}$ (1_{A_k} is the characteristic function on A_k), and for these functions, we define

$$\int_{\Omega} f(x) d\mu(x) = \sum_{k=1}^{n} \mu(A_k) x_k$$

where $A_k \in \mathcal{A}$, and $x_k \in \mathcal{X}$.

Definition 1.4.1. *A function $f : \Omega \to \mathcal{X}$ is μ-Bochner integrable if there exists a sequence of μ-simple functions $f_n : \Omega \to \mathcal{X}$ such that the following two conditions are hold*

$$(i) \lim_{n\to\infty} f_n(x) = f(x) \quad \mu - \textit{almost everywhere, and} \tag{1.6}$$

$$(ii) \lim_{n\to\infty} \|f_n - f\| d\mu = 0. \tag{1.7}$$

If f is μ-Bochner integrable, then

$$\int_{\Omega} f(x) d\mu(x) = \lim_{n\to\infty} \int_{\Omega} f_n(x) d\mu(x).$$

Another equivalent condition for Bochner integrability is given in the following proposition.

Proposition 1.4.2. *[28, Prposition 1.2.2] A strongly μ-measurable function $f : A \to \mathcal{X}$ is μ-Bochner integrable if and only if*

$$\int_A \|f\| d\mu < \infty,$$

and in this case we have

$$\|\int_A f d\mu\| \leq \int_A \|f\| d\mu.$$

The analogue result of dominate convergence theorem (DCT) is also available here. The result is as follows.

Theorem 1.4.3. *[28, Prposition 1.2.5] Let $f_n : A \to \mathcal{X}$ be sequence of functions, each of which is the μ-Bochner integrable. Assume that there exist a function $f : A \to \mathcal{X}$ and a μ-integrable function g such that*
(i) $\lim_{n\to\infty} f_n(x) = f(x)$ $\mu -$ almost everywhere
(ii) $\|f_n\| \leq |g|$ $\mu -$ almost everywhere.
Then f is μ-Bochner integrable, and

$$\lim_{n\to\infty} \int_A f_n d\mu = \int_A f d\mu.$$

Now we are providing a very useful result due to Duhamel, and the proof of this result can be found in [5, Lemma 5.2].

Lemma 1.4.4 (Duhamel's Formula). *If H_0 is a self-adjoint operator in $\mathcal{H}$, $V = V^* \in \mathcal{B}(\mathcal{H})$ and if $H = H_0 + V$, then*

$$e^{isH} - e^{isH_0} = \int_0^s e^{i(s-t)H} iV e^{itH_0} dt, s \in \mathbb{R},$$

where the integral in the right hand side is a Bochner integral and it converges in the strong operator topology.

Next we introduce some needful function spaces.

1.5 Function spaces

Let $n \in \mathbb{N}$. Let us consider the following class of functions

$$\begin{aligned}
\mathcal{F}_n(\mathbb{T}) &:= \left\{\phi \mid \phi : \mathbb{T} \to \mathbb{C},\ \phi(z) = \sum_{k=-\infty}^{\infty} a_k z^k \text{ with } \sum_{k=-\infty}^{\infty} |k|^n |a_k| < \infty\right\}, \\
\mathcal{F}_n^+(\mathbb{T}) &:= \left\{\phi \mid \phi : \mathbb{T} \to \mathbb{C},\ \phi(z) = \sum_{k=0}^{\infty} a_k z^k \text{ with } \sum_{k=0}^{\infty} k^n |a_k| < \infty\right\}, \\
\mathcal{F}_{nn}^+(\mathbb{T}) &:= \left\{\phi \mid \phi : \mathbb{T} \to \mathbb{C},\ \phi(z) = \sum_{k=n}^{\infty} a_k z^k \text{ with } \sum_{k=n}^{\infty} k^n |a_k| < \infty\right\}, \\
\mathcal{F}_n^+(\mathbb{R}) &:= \left\{\psi : \mathbb{R} \to \mathbb{C} \text{ such that } \psi(\lambda) = \phi\left(\frac{i-\lambda}{i+\lambda}\right) \text{ for some } \phi \in \mathcal{F}_n^+(\mathbb{T})\right\}, \\
\mathcal{F}_{nn}^+(\mathbb{R}) &:= \left\{\psi : \mathbb{R} \to \mathbb{C} \text{ such that } \psi(\lambda) = \phi\left(\frac{i-\lambda}{i+\lambda}\right) \text{ for some } \phi \in \mathcal{F}_{nn}^+(\mathbb{T})\right\}.
\end{aligned} \tag{1.8}$$

Let X be a non-empty subset of $\mathbb{R}$ (or $\mathbb{T}$) possibly coinciding with $\mathbb{R}$ (or $\mathbb{T}$). Let $B(X)$ denote the space of all bounded functions on X, $C(X)$ the space of all continuous functions on X, $C_0(\mathbb{R})$ the space of continuous functions on $\mathbb{R}$ decaying to 0 at infinity, $C^n(X)$ the space of n-times continuously differentiable functions on X. Let $C_b^n(X)$ denote the subset of $C^n(X)$ of such f for which $f^{(n)}$ is bounded. Let $C_c^n(\mathbb{R})$ denote the subspace of $C^n(\mathbb{R})$ consisting of compactly supported functions. We also use the notation $C^0(\mathbb{R}) = C(\mathbb{R})$. Let $a, b \in \mathbb{R}$. Let $C_c^n((a,b))$ denote the subspace of $C_c^n(\mathbb{R})$ consisting of the functions whose closed support is contained in (a,b), let $D_c^n((a,b))$ denote the space of n-times differentiable functions in $C_c((a,b))$, and let $F_c^n((a,b))$ denote the subspace of $C_c^{n-1}((a,b))$ consisting of f such that $f^{(n)}$ exists almost everywhere in (a,b) and $f^{(n)} \in L^2((a,b))$. We note that for every $f \in F_c^n((a,b))$ the function $f^{(n-1)}$ is absolutely continuous. We write $f(x) = o(g(x))$ if for all $\epsilon > 0$, we have $|f(x)| \le \epsilon g(x)$ for all x outside a compact set depending on ϵ.

Given $f \in L^1(\mathbb{R})$ (or $L^1(\mathbb{T})$), let $\hat{f}$ denote the Fourier transform of f. We will use the well-known property that every $f \in C_c^n(\mathbb{R})$ satisfies $\widehat{f^{(n-1)}} \in L^1(\mathbb{R})$.

Divided Differences: Let $f \in C^n(\mathbb{R})$. Recall that the divided difference of order n is an operation on the function f of one (real) variable, and is defined recursively as follows:

$$f^{[0]}(\lambda) = f(\lambda),$$

$$f^{[n]}(\lambda_0, \lambda_1, \ldots, \lambda_n) = \begin{cases} \frac{f^{[n-1]}(\lambda_0,\lambda_1,\ldots,\lambda_{n-2},\lambda_n) - f^{[n-1]}(\lambda_0,\lambda_1,\ldots,\lambda_{n-2},\lambda_{n-1})}{\lambda_n - \lambda_{n-1}} & \text{if } \quad \lambda_n \neq \lambda_{n-1}, \\ \frac{\partial}{\partial \lambda} f^{[n-1]}(\lambda_0, \lambda_1, \ldots, \lambda_{n-2}, \lambda)\Big|_{\lambda=\lambda_{n-1}} & \text{if } \quad \lambda_n = \lambda_{n-1}. \end{cases}$$

Functions of contraction: Let $\phi \in \mathcal{F}_1(\mathbb{T})$ (see (1.8)) be such that $\phi(e^{it}) = \sum_{k=-\infty}^{\infty} \hat{\phi}(k)e^{ikt}$. Now we introduce the functions, namely $\phi_+(e^{it}) = \sum_{k=0}^{\infty} \hat{\phi}(k)e^{ikt}$ and $\phi_-(e^{it}) = \sum_{k=1}^{\infty} \hat{\phi}(-k)e^{ikt}$. Then $\phi(e^{it}) = \phi_+(e^{it}) + \phi_-(e^{-it})$ and $\phi_\pm \in \mathcal{F}_2^+(\mathbb{T})$. Thus for a given contraction T on $\mathcal{H}$, we set

$$\begin{aligned} &\phi_+(T) = \sum_{k=0}^{\infty} \hat{\phi}(k)T^k, \ \phi_-(T) = \sum_{k=1}^{\infty} \hat{\phi}(-k)T^{*k}, \text{ and} \\ &\phi(T) = \phi_+(T) + \phi_-(T). \end{aligned} \tag{1.9}$$

1.6 Dilation Theory

Definition 1.6.1. *Let T be a bounded operator on $\mathcal{H}$. We say T has a unitary dilation if there exists a Hilbert space $\mathcal{K}$ containing $\mathcal{H}$ as a subspace, and a unitary operator U_T on $\mathcal{K}$ such that*

$$T^n = P_{\mathcal{H}} U_T^n\big|_{\mathcal{H}}, \ \text{and } T^{-n} := T^{*n} = P_{\mathcal{H}} U_T^{*n}\big|_{\mathcal{H}}, \tag{1.10}$$

where $P_{\mathcal{H}} : \mathcal{K} \to \mathcal{H}$ is the orthogonal projection. U_T is called the minimal dilation of T if

$$\mathcal{K} = \bigvee_{k\in\mathbb{Z}} U_T^k \mathcal{H}.$$

It is clear from (1.10) that if T has a unitary dilation, then T must be a contraction and also T has the minimal unitary dilation with minimal dilation space $\mathcal{K} = \bigvee_{k\in\mathbb{Z}} U_T^k \mathcal{H}$. It is well known that the converse is also true; that is, every contraction has a unitary dilation. Here we give an explicit construction of a unitary dilation, known as Schäffer matrix unitary dilation, associated with a given contraction. For that, consider the two-sided sequence space $l^2_{\mathbb{Z}}(\mathcal{H})$ of $\mathcal{H}$-valued sequences by

$$l^2_{\mathbb{Z}}(\mathcal{H}) := \bigoplus_{n=-\infty}^{-1} \mathcal{H} \bigoplus \mathcal{H} \bigoplus_{n=1}^{\infty} \mathcal{H}.$$

Note that we embed $\mathcal{H}$ in $l^2_{\mathbb{Z}}(\mathcal{H})$ by identifying the element $h \in \mathcal{H}$ with the vector $\{h_n\}_{n\in\mathbb{Z}} \in l^2_{\mathbb{Z}}(\mathcal{H})$ for which $h_0 = h$ and $h_n = 0$ $(n \neq 0)$. Then $\mathcal{H}$ becomes a subspace of $l^2_{\mathbb{Z}}(\mathcal{H})$, and the orthogonal projection from $l^2_{\mathbb{Z}}(\mathcal{H})$ into $\mathcal{H}$ is given by

$$P_{\mathcal{H}}(\{h_n\}_{n\in\mathbb{Z}}) = h_0. \tag{1.11}$$

The Schäffer matrix unitary dilation U_T of T on the two-sided sequence space $l^2_{\mathbb{Z}}(\mathcal{H})$ is given by

$$U_{_T} = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & ⋰ \\ \cdots & 0 & 0 & I & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & D_T & -T^* & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & \boxed{T} & D_{T^*} & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & 0 & I & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & 0 & 0 & I & \cdots \\ ⋰ & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \tag{1.12}$$

where $D_T = (I - T^*T)^{1/2}$ and $D_{T^*} = (I - TT^*)^{1/2}$ are the defect operators corresponding to the contractions T and T^* respectively. In the block matrix representation (1.12) of U_T, the entry T is at the $(0,0)$ position and the (i,j)-th entries $U_{_T}(i,j)$ of $U_{_T}$ are given by

$$U_{_T}(0,0) = T,\ U_{_T}(-1,0) = D_T,\ U_{_T}(-1,1) = -T^*,\ U_{_T}(0,1) = D_{T^*},\ U_{_T}(j,j+1) = I$$

for $j \neq 0, -1$, while all the remaining entries are equal to zero.

It is important to note that such a dilation does not have to be minimal but at the same time the advantage of this dilation is that it allows us to consider unitary dilations of contractions on $\mathcal{H}$ on the same Hilbert space $l^2_{\mathbb{Z}}(\mathcal{H})$. The minimal dilation space of the above unitary dilation is $\bigoplus\limits_{n=-\infty}^{-1} \mathcal{D}_T \bigoplus \mathcal{H} \bigoplus\limits_{n=1}^{\infty} \mathcal{D}_{T^*}$. We refer [70, Chapter I] for more information regarding unitary dilations.

1.6.1 Semi-spectral measure

A *semi-spectral measure* $\mathcal{E}$ on a measurable space $(\mathcal{X}, \mathcal{B})$ is a map on the σ-algebra $\mathcal{B}$ with values in the set of bounded linear operators on a Hilbert space $\mathcal{H}$ that is countably additive in the strong operator topology and such that

$$\mathcal{E}(\Delta) \geq 0 \text{ for all } \Delta \in \mathcal{B},\ \mathcal{E}(\emptyset) = 0,\ \text{and } \mathcal{E}(\mathcal{X}) = I.$$

It is interesting to observe that by Naimark's theorem [43] each semi-spectral measure $\mathcal{E}$ has a *spectral dilation*, that is a spectral measure E on the same measurable space $(\mathcal{X}, \mathcal{B})$ that takes values in the set of orthogonal projections on a Hilbert space $\mathcal{K}$ containing $\mathcal{H}$, and such that

$$\mathcal{E}(\Delta) = P_{\mathcal{H}} E(\Delta)|_{\mathcal{H}}, \quad \Delta \in \mathcal{B},$$

where $P_{\mathcal{H}}$ is the orthogonal projection on $\mathcal{K}$ onto $\mathcal{H}$. Integrals with respect to semi-spectral measures are defined in the following way:

$$\int_{\mathcal{X}} \phi(x)\ \mathcal{E}(dx) = P_{\mathcal{H}} \left(\int_{\mathcal{X}} \phi(x)\ E(dx) \right) \Big|_{\mathcal{H}}, \quad \phi \in L^\infty(E).$$

Recall that each contraction T (that is, $\|T\| \le 1$) on a Hilbert space $\mathcal{H}$ has a minimal unitary dilation U, that is U is a unitary operator on a Hilbert space $\mathcal{K}$, $\mathcal{H} \subseteq \mathcal{K}$, $T^n = P_{\mathcal{H}} U^n|_{\mathcal{H}}$ for $n \ge 0$ and $\mathcal{K}$ is the closed linear span of $U^n\mathcal{H}$, $n \in \mathbb{Z}$ (see [70], Ch. I, Theorem 4.2). Here $P_{\mathcal{H}}$ is the orthogonal projection on $\mathcal{K}$ onto $\mathcal{H}$. The *semi-spectral measure* $\mathcal{E}_T$ of T is defined by

$$\mathcal{E}_T(\Delta) \stackrel{\text{def}}{=} P_{\mathcal{H}} E_U(\Delta)|_{\mathcal{H}}, \tag{1.13}$$

where $\int_0^{2\pi} e^{it}\ E_U(dt)$ is the spectral representation of U, $E_U(\cdot)$ is the spectral measure determined uniquely by the unitary operator U such that it is continuous at $t = 0$, that is, $E_U(0) = 0$ (see page 281, [58]), and Δ is a Borel subset of $[0, 2\pi]$. Then it is easy to see that

$$T^n = \int_0^{2\pi} e^{int}\ \mathcal{E}_T(dt), \quad n \in \mathbb{N} \cup \{0\}. \tag{1.14}$$

For more on semi-spectral measures and related stuff, we refer to [3].

CHAPTER 2

Koplienko-Neidhardt trace formula for unitaries – A new proof

2.1 Introduction

One of the fundamental concept in perturbation theory is the existence of spectral shift function and the associated trace formula. The notion of first order spectral shift function originated from Lifshits' work on theoretical physics [35] and later the mathematical theory of this object elaborated by M.G. Krein in a series of papers, starting with [32]. In [32] (see also [34]), Krein proved that given two self-adjoint operators H and H_0 (possibly unbounded) such that $H - H_0$ is trace class, then there exists a unique real valued $L^1(\mathbb{R})$ function ξ such that

$$\text{Tr}\ \{\phi(H) - \phi(H_0)\} = \int_{\mathbb{R}} \phi'(\lambda)\ \xi(\lambda)\ d\lambda \tag{2.1}$$

holds for sufficiently nice functions ϕ. The function ξ is known as Krein's spectral shift function and the relation (2.1) is called Krein's trace formula. The original proof of Krein uses analytic function theory. Later in [12] (see also [10]), Birman and Solomyak approached the trace formula (2.1) using the theory of double operator integrals, though they failed to prove the absolute continuity of the spectral shift. In 1985, Voiculescu [74] gave an alternative proof of the trace formula (2.1) by adapting the proof of classical Weyl-von Neumann theorem for the case of bounded self-adjoint operators and later Sinha and Mohapatra extended Voiculescu's method to the unbounded self-adjoint case [63]. A similar result was obtained by Krein in [33] for pair of unitary operators $\{U, U_0\}$ such that $U - U_0$ is trace class. For each such pair there exists a real valued $L^1([0, 2\pi])$- function ξ, unique modulo an additive constant, (called a spectral shift function for $\{U, U_0\}$) such that

$$\operatorname{Tr}\left\{\phi(U) - \phi(U_0)\right\} = \int_0^{2\pi} \frac{d}{dt}\left\{\phi(e^{it})\right\} \xi(t)\, dt, \tag{2.2}$$

whenever ϕ' has absolutely convergent Fourier series. Later in [41], Sinha and Mohapatra also obtained the above formula (2.2) using Voiculescu's method. Recently, Aleksandrov and Peller [2] extended the formula (2.2) for arbitrary operator Lipschitz functions ϕ on the unit circle $\mathbb{T}$. Moreover, Peller [51] describe completely the class of functions (viz, the class of operator Lipschitz functions on $\mathbb{R}$), for which the Krein's trace formula (2.1) holds. We refer to [36, 39, 38, 59, 60, 61, 62] for more on the Krein trace formula for pairs of arbitrary contractions.

The modified second order spectral shift function for Hilbert-Schmidt perturbations was introduced by Koplienko in [31]. Let H and H_0 be two self-adjoint operators in a separable Hilbert space $\mathcal{H}$ such that $H - H_0 = V \in \mathcal{B}_2(\mathcal{H})$. Sometimes H_0 is known as the initial operator, V is known as the perturbation operator, and $H = H_0 + V$ is known as the final operator. In this case the difference $\phi(H) - \phi(H_0)$ is no longer of trace-class and one has to consider instead

$$\phi(H) - \phi(H_0) - \frac{d}{ds}\Big(\phi(H_0 + sV)\Big)\Big|_{s=0},$$

where $\frac{d}{ds}\Big(\phi(H_0 + sV)\Big)\Big|_{s=0}$ denotes the Gâteaux derivative of ϕ at H_0 in the direction V (see [8]) and and find a trace formula for the above expression under certain assumptions on ϕ. Under the above hypothesis, Koplienko's formula asserts that there exists a unique function $\eta \in L^1(\mathbb{R})$ such that

$$\operatorname{Tr}\left\{\phi(H) - \phi(H_0) - \frac{d}{ds}\Big(\phi(H_0 + sV)\Big)\Big|_{s=0}\right\} = \int_{\mathbb{R}} \phi''(\lambda)\, \eta(\lambda)\, d\lambda \tag{2.3}$$

for rational functions ϕ with poles off $\mathbb{R}$. The function η is known as Koplienko spectral shift function corresponding to the pair (H_0, H). In 2007, Gesztesy, Pushnitski and Simon [26] gave an alternative proof of the formula (2.3) for the bounded case and in 2009, Dykema and Skripka [23, 64], and earlier Boyadzhiev [13] obtained the formula (2.3) in the semi-finite von Neumann algebra setting. Later in 2012, Sinha and Chattopadhyay provide an alternative proof of the formula (2.3) using the idea of finite dimensional approximation method as in the works of Voiculescu [74], Sinha and Mohapatra [63, 41]. In this connection it is worth mentioning that in 1984, Koplienko also conjectured about the existence of the higher order spectral shift measures ν_n, $n > 2$, for the perturbation $V \in \mathcal{B}_n(\mathcal{H})$ and it is remarkable to note that recently Potapov, Skripka and Sukochev resolve affirmatively Koplienko's conjecture and establishes the existence of higher order spectral shift function in their outstanding and beautiful paper [53] using the concept of multiple operator integral.

A similar problem for unitary operators was considered by Neidhardt [42]. Let U and U_0 be two unitary operators on a separable Hilbert space $\mathcal{H}$ such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$. Then $U = e^{iA}U_0$, where A is a self-adjoint operator in $\mathcal{B}_2(\mathcal{H})$. Note that we interpret U_0 as the initial operator, A as the perturbation operator, and $U = e^{iA}U_0$ as the final operator. Denote $U_s = e^{isA}U_0$, $s \in \mathbb{R}$. Then it was shown in [42] that there exists a $L^1([0, 2\pi]))$-function η (unique upto an additive constant) such that

$$\operatorname{Tr}\left\{\phi(U) - \phi(U_0) - \frac{d}{ds}\phi(U_s)\Big|_{s=0}\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\{\phi(e^{it})\}\eta(t)dt, \tag{2.4}$$

whenever ϕ'' has absolutely convergent Fourier series. The function η is known as Koplienko spectral shift function corresponding to the pair (U_0, U). In [48], Peller obtained better sufficient conditions on functions ϕ, under which trace formulae (2.3) and (2.4) hold. In this connection, it is also worth mentioning that recently Potapov, Skripka and Sukochev proved higher order analogs of the formula (2.4) in [55]. For more about trace formulas and related topics, we refer the reader to ([37, 38, 39, 47, 49, 52, 54, 56, 66, 69]) and the references cited therein.

In this chapter we once again supply the new proof of the Koplienko-Neidhardt trace formula (2.4), we believe for the first time, using the idea of finite dimensional approximation method as in the works of Voiculescu, Sinha and Mohapatra, referred earlier. The major differences between our method and the method applied in [31, 42] are the following.

(a) In [31, 42], the authors have reduced the problem by truncating only the perturbation operator (and not the initial operator) via finite rank projections but still, they were in an infinite-dimensional setting to deal with the problem which makes a major contrast in comparison to our context. In other words, in our setting, we reduce the problem into a finite dimensional one by truncating both the initial operator and the perturbation operator simultaneously via finite dimensional projections $\{P_n\}$ obtained by Weyl-von Neumann type construction (see Lemma 2.3.1). Moreover, the authors have obtained the expression of the shift function in [31, 42] for the reduced system as a consequence of Theorem 3 of [10] and Krein's spectral shift function whereas in our context we calculate the shift function explicitly by performing integration by-parts and using spectral theorem for unitary matrices (see Theorem 2.2.2).

(b) A concept like the continuity of the perturbation determinant has been used in [31, 42] to approximate the formula in infinite dimension but in our setting we do not need it to get the required approximation (see Theorem 2.3.6).

(c) In [31, 42], the authors dealt with the dual of $C([0,2\pi])$ $\big($set of all continuous functions defined on $[0,2\pi]$ $\big)$ to get the shift function in an infinite dimension whereas we use pre-dual of $L^\infty([0,2\pi])$ $\big($set of all bounded measurable functions defined on $[0,2\pi]\big)$ to get the same (see Theorem 2.4.1$\big)$.

The rest of the chapter is organized as follows: In Section 2.2, we give a proof of the Koplienko-Neidhardt trace formula when $dim\ \mathcal{H} < \infty$. Section 2.3 is devoted to the reduction of the problem to finite dimensions and in Section 2.4 we prove the trace formula by a limiting argument.

2.2 Koplienko-Neidhardt trace formula in finite dimension

Here, $\mathcal{H}$ will denote the separable Hilbert space we work in; $\mathcal{B}(\mathcal{H})$, $\mathcal{B}_1(\mathcal{H})$, $\mathcal{B}_2(\mathcal{H})$ the set of bounded, trace class, Hilbert-Schmidt class operators in $\mathcal{H}$ respectively with $\|\cdot\|, \|\cdot\|_1, \|\cdot\|_2$ as the associated norms and $\mathrm{Tr}\{A\}$ denote the trace of a trace class operator A (see Chapter 1 for notations).

Theorem 2.2.1. *Let U and U_0 be two unitary operators on a separable Hilbert space $\mathcal{H}$ such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$. Then there exists a self-adjoint operator $A \in \mathcal{B}_2(\mathcal{H})$ such that $U = e^{iA}U_0$.*

Proof. Since UU_0^* is a unitary operator, then there is a self-adjoint operator A with the spectrum in $(-\pi,\pi]$ (that is, $\sigma(A) \subseteq (-\pi,\pi]$) such that $UU_0^* = e^{iA}$ and hence $U = e^{iA}U_0$. Let $\{f_i\}$ be any orthonormal basis of $\mathcal{H}$. Then from the inequality $|x| \leq \frac{\pi}{2}|e^{ix}-1|$ for $x \in (-\pi,\pi]$ and by using the spectral theorem (see Theorem 1.2.14) we conclude

$$\begin{aligned} ||A||_2^2 = \sum_{i=1}^{\infty} ||Af_i||^2 = \sum_{i=1}^{\infty} \int_{-\pi}^{\pi} |\lambda|^2 \; ||E(d\lambda)f_i||^2 \leq \frac{\pi^2}{4} \sum_{i=1}^{\infty} \int_{-\pi}^{\pi} |e^{i\lambda}-1|^2 \; ||E(d\lambda)f_i||^2 \\ = \frac{\pi^2}{4} \left\|e^{iA}-I\right\|_2^2 = \frac{\pi^2}{4}\|U-U_0\|_2^2, \end{aligned}$$

where $E(\cdot)$ is the spectral measure corresponding to the self-adjoint operator A. Thus from the hypothesis we conclude that $A \in \mathcal{B}_2(\mathcal{H})$. This completes the proof. □

The following theorem states Koplienko-Neidhardt trace formula in finite dimension.

Theorem 2.2.2. *Let U and U_0 be two unitary operators in a separable Hilbert space $\mathcal{H}$ such that $U-U_0 \in \mathcal{B}_2(\mathcal{H})$ and $p(\lambda)=\lambda^r$ $(r \in \mathbb{Z})$, $\lambda \in \mathbb{T}$.*

(i) Then

$$\frac{d}{ds}(p(U_s)) = \begin{cases} \sum_{k=0}^{r-1} U_s^{r-k-1} \; (iA) \; U_s^{k+1} & \text{if } r \geq 1, \\ 0 & \text{if } r=0, \\ -\sum_{k=0}^{|r|-1} (U_s^*)^{|r|-k} \; (iA) \; (U_s^*)^k & \text{if } r \leq -1, \end{cases} \tag{2.5}$$

where $U_s = e^{isA}U_0$, $s \in \mathbb{R}$.

(ii) If furthermore $\dim(\mathcal{H}) < \infty$, then

$$p(U)-p(U_0)-\frac{d}{ds}(p(U_s))\Big|_{s=0} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists a $L^1([0,2\pi])$- function η (unique upto an additive constant) such that

$$\operatorname{Tr}\left\{p(U)-p(U_0)-\frac{d}{ds}(p(U_s))\Big|_{s=0}\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\{p(e^{it})\} \; \eta(t) \; dt, \tag{2.6}$$

where $p(\cdot)$ is any trigonometric polynomial on $\mathbb{T}$ with complex coefficients and

$$\eta(t) = \int_0^1 \operatorname{Tr}\{A[E_0(t)-E_s(t)]\} ds \;, \quad t \in [0,2\pi] \tag{2.7}$$

where $E_s(\cdot)$ is the spectral measure of the unitary operator U_s. Moreover,

$$\operatorname{Tr}\left\{p(U)-p(U_0)-\frac{d}{ds}(p(U_s))\Big|_{s=0}\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\{p(e^{it})\} \; \eta_o(t) \; dt, \tag{2.8}$$

where

$$\eta_o(t) = \eta(t) - \frac{1}{2\pi}\int_0^{2\pi} \eta(s)ds \;, \quad t \in [0,2\pi] \quad \text{and} \quad \|\eta_o\|_{L^1([0,2\pi])} \leq \frac{\pi}{2}\|A\|_2^2.$$

Proof. (i) Since $U - U_0 \in \mathcal{B}_2(\mathcal{H})$, then by the above Theorem 2.2.1 there exists a self-adjoint operator $A \in \mathcal{B}_2(\mathcal{H})$ such that $U = e^{iA}U_0$. Denote $U_s = e^{isA}U_0,\ s \in \mathbb{R}$ and note that each U_s is an unitary operator. For $p(\lambda) = \lambda^r\ (r \geq 1),\ \lambda \in \mathbb{T}$, we have

$$\frac{p(U_{s+h}) - p(U_s)}{h} = \frac{1}{h}\sum_{k=0}^{r-1} U_{s+h}^{r-k-1}\left[U_{s+h} - U_s\right] U_s^k = \frac{1}{h}\sum_{k=0}^{r-1} U_{s+h}^{r-k-1}\left[e^{ihA} - I\right] U_s^{k+1},$$

which converges in operator norm to

$$\sum_{k=0}^{r-1} U_s^{r-k-1}\,(iA)\,U_s^{k+1} \quad \text{as} \quad h \to 0.$$

Similarly for $p(\lambda) = \lambda^r\ (r \leq -1),\ \lambda \in \mathbb{T}$, we have

$$\begin{aligned}\frac{p(U_{s+h}) - p(U_s)}{h} &= \frac{1}{h}\sum_{k=0}^{|r|-1} (U_{s+h}^*)^{|r|-k-1}\left[U_{s+h}^* - U_s^*\right](U_s^*)^k\\ &= \frac{1}{h}\sum_{k=0}^{|r|-1} (U_{s+h}^*)^{|r|-k-1}(U_s^*)\left[e^{-ihA} - I\right](U_s^*)^k,\end{aligned}$$

which again converges in operator norm to

$$-\sum_{k=0}^{r-1} (U_s^*)^{|r|-k}(iA)(U_s^*)^k \quad \text{as} \quad h \to 0.$$

(ii) By using the cyclicity of trace and noting that the trace now is a finite sum, we have that for $p(\lambda) = \lambda^r\ (r \geq 1),\ \lambda \in \mathbb{T}$,

$$\begin{aligned}&\mathrm{Tr}\left\{p(U) - p(U_0) - \frac{d}{ds}p(U_s)\Big|_{s=0}\right\} = \mathrm{Tr}\left\{\int_0^1 \frac{d}{ds}(p(U_s))\,ds\right\} - \mathrm{Tr}\left\{\frac{d}{ds}p(U_s)\Big|_{s=0}\right\}\\ &= \int_0^1 \mathrm{Tr}\left\{\sum_{k=0}^{r-1} U_s^{r-k-1}\,(iA)\,U_s^{k+1}\right\} ds - \mathrm{Tr}\left\{\sum_{k=0}^{r-1} U_0^{r-k-1}\,(iA)\,U_0^{k+1}\right\}\\ &= \int_0^1 r\ \mathrm{Tr}\left(iAU_s^r\right) ds - \int_0^1 r\ \mathrm{Tr}\left(iAU_0^r\right) ds = \mathrm{Tr}\left\{r(iA)\int_0^1 ds \int_0^{2\pi} e^{irt}\big(E_s(dt) - E_0(dt)\big)\right\},\end{aligned}$$

where $E_s(\cdot)$ and $E_0(\cdot)$ are the spectral measures determined uniquely by the unitary operators U_s and U_0 respectively such that the spectral measures are continuous at $t = 0$, that is, $E_s(0) = 0 = E_0(0)$ (see Theorem 1.2.15). Next by performing integration by-parts we have that

$$\mathrm{Tr}\left\{p(U) - p(U_0) - \frac{d}{ds}p(U_s)\Big|_{s=0}\right\}$$

$$= \text{Tr}\left\{r(iA)\int_0^1 ds\, \left(e^{irt}\big[E_s(t)-E_0(t)\big]\Big|_{t=0}^{2\pi} - ir\int_0^{2\pi} e^{irt}\big[E_s(t)-E_0(t)\big]dt\right)\right\}$$
$$= \int_0^{2\pi}(ir)^2 e^{irt}\left(\int_0^1 \text{Tr}\left\{A[E_0(t)-E_s(t)]\right\}ds\right) = \int_0^{2\pi}\frac{d^2}{dt^2}[p(e^{it})]\,\eta(t)\,dt,$$

where we have set

$$\eta(t) = \int_0^1 \text{Tr}\left\{A[E_0(t)-E_s(t)]\right\}ds.$$

In similar manner, we can prove the identity (2.6) for $p(\lambda)=\lambda^r\ (r\leq -1),\ \lambda\in\mathbb{T}$. Indeed, let $p(\lambda)=\lambda^r\ (r\leq -1),\ \lambda\in\mathbb{T}$. Then

$$\text{Tr}\left\{p(U)-p(U_0)-\frac{d}{ds}p(U_s)\Big|_{s=0}\right\} = \text{Tr}\left\{\int_0^1\frac{d}{ds}(p(U_s))\,ds\right\} - \text{Tr}\left\{\frac{d}{ds}p(U_s)\Big|_{s=0}\right\}$$
$$= \int_0^1 \text{Tr}\left\{\sum_{k=0}^{|r|-1}(U_s^*)^{|r|-k}\,(-iA)\,(U_s^*)^k\right\}ds - \text{Tr}\left\{\sum_{k=0}^{|r|-1}(U_0^*)^{|r|-k}\,(-iA)\,(U_0^*)^k\right\}$$
$$= -\int_0^1 |r|\ \text{Tr}\left(iA(U_s^*)^{|r|}\right)ds + \int_0^1 |r|\ \text{Tr}\left(iA(U_0^*)^{|r|}\right)ds$$
$$= \text{Tr}\left\{|r|(iA)\int_0^1 ds\ \int_0^{2\pi} e^{-i|r|t}\big(E_0(dt)-E_s(dt)\big)\right\},$$

Next by performing integration by-parts we have that

$$\text{Tr}\left\{p(U)-p(U_0)-\frac{d}{ds}p(U_s)\Big|_{s=0}\right\}$$
$$= \text{Tr}\left\{|r|(iA)\int_0^1 ds\,\left(e^{-i|r|t}\big[E_0(t)-E_s(t)\big]\Big|_{t=0}^{2\pi} + i|r|\int_0^{2\pi}e^{-i|r|t}\big[E_0(t)-E_s(t)\big]dt\right)\right\}$$
$$= \int_0^{2\pi}(i|r|)^2 e^{-i|r|t}\left(\int_0^1 \text{Tr}\left\{A[E_0(t)-E_s(t)]\right\}ds\right) = \int_0^{2\pi}\frac{d^2}{dt^2}[p(e^{it})]\,\eta(t)\,dt,$$

Now it is clear that $\eta \in L^1([0,2\pi])$ and therefore it makes sense to define

$$\eta_o(t) = \eta(t) - \frac{1}{2\pi}\int_0^{2\pi}\eta(s)ds, \quad t\in[0,2\pi].$$

Thus the assertion (2.8) follows from the following observation

$$\int_0^{2\pi} e^{imt}\eta_0(t) = \int_0^{2\pi} e^{imt}\left[\eta(t) - \frac{1}{2\pi}\int_0^{2\pi}\eta(s)ds\right]dt$$
$$= \int_0^{2\pi} e^{imt}\eta(t)dt - \frac{1}{2\pi}\int_0^{2\pi}\eta(s)ds\int_0^{2\pi}e^{imt}dt$$
$$= \int_0^{2\pi} e^{imt}\eta(t)dt \quad \text{for} \quad m\in\mathbb{Z}\setminus\{0\}.$$

Let $f\in L^\infty([0,2\pi])$, and consider

$$f_o = f - \frac{1}{2\pi}\int_0^{2\pi} f(s)ds.$$

Then it is easy to observe that

$$\int_0^{2\pi} f(t)\eta_o(t)dt = \int_0^{2\pi} f_o(t)\eta(t)dt, \quad \int_0^{2\pi} f_o(t)dt = 0, \quad \text{and} \quad \|f_o\|_\infty \leq 2\|f\|_\infty.$$

Therefore by using the expression (2.7) of η and using Fubini's theorem to interchange the orders of integration and integrating by-parts, we have for $g(e^{it}) = \int_0^t f_0(s)ds, t \in [0, 2\pi]$ that

$$\begin{aligned}
&\int_0^{2\pi} f(t)\eta_o(t)dt = \int_0^{2\pi} f_o(t)\eta(t)dt = \int_0^{2\pi} \frac{d}{dt}[g(e^{it})] \left(\int_0^1 \mathrm{Tr}[A(E_0(t) - E_s(t))]ds\right) dt \\
&= \int_0^1 ds \int_0^{2\pi} \frac{d}{dt}[g(e^{it})] \,\mathrm{Tr}[A(E_0(t) - E_s(t))]dt \\
&= \int_0^1 ds \left\{ g(e^{it})\,\mathrm{Tr}[A(E_0(t) - E_s(t))]\Big|_{t=0}^{2\pi} - \int_0^{2\pi} g(e^{it})\,\mathrm{Tr}[A(E_0(dt) - E_s(dt))] \right\} \\
&= -\int_0^1 ds \int_0^{2\pi} g(e^{it})\,\mathrm{Tr}[A(E_0(dt) - E_s(dt))] = \int_0^1 \mathrm{Tr}[A\{g(U_s) - g(U_0)\}]ds. \qquad (2.9)
\end{aligned}$$

On the other hand by using the idea of double operator integrals (see Definition 1.3.1), introduced by Birman and Solomyak [10, 12, 11] we have

$$\begin{aligned}
g(U_s) - g(U_0) &= \int_0^{2\pi}\int_0^{2\pi} \left[g(e^{i\lambda}) - g(e^{i\mu})\right] E_s(d\lambda)E_0(d\mu) \\
&= \int_0^{2\pi}\int_0^{2\pi} \frac{g(e^{i\lambda}) - g(e^{i\mu})}{e^{i\lambda} - e^{i\mu}} E_s(d\lambda)(U_s - U_0)E_0(d\mu) \\
&= \int_0^{2\pi}\int_0^{2\pi} \frac{g(e^{i\lambda}) - g(e^{i\mu})}{e^{i\lambda} - e^{i\mu}} \mathcal{G}(d\lambda \times d\mu)(U_s - U_0), \qquad (2.10)
\end{aligned}$$

where $\mathcal{G}(\Delta \times \delta)(V) = E_s(\Delta)VE_0(\delta)$ ($V \in \mathcal{B}_2(\mathcal{H})$ and $\Delta \times \delta \subseteq \mathbb{R} \times \mathbb{R}$) extends to a spectral measure on $\mathbb{R}^2$ in the Hilbert space $\mathcal{B}_2(\mathcal{H})$ (equipped with the inner product derived from the trace) and its total variation is less than or equal to $\|V\|_2$. Thus by using the standard inequality $\left|\frac{g(e^{i\lambda}) - g(e^{i\mu})}{e^{i\lambda} - e^{i\mu}}\right| \leq \frac{\pi}{2}\|f_o\|_\infty \leq \pi\|f\|_\infty$, for $\lambda, \mu \in [0, 2\pi]$, we conclude from (2.10) that

$$\|g(U_s) - g(U_0)\|_2 \leq \pi\|f\|_\infty\|U_s - U_0\|_2, \qquad (2.11)$$

which combining with (2.9) implies that

$$\begin{aligned}
&\left|\int_0^{2\pi} f(t)\eta_o(t)dt\right| \leq \int_0^1 \|A\|_2\, \|g(U_s) - g(U_0)\|_2\, ds \leq \pi\|f\|_\infty\|A\|_2 \int_0^1 \|U_s - U_0\|_2\, ds \\
&\leq \pi\|f\|_\infty\|A\|_2 \int_0^1 s\|A\|_2\, ds = \frac{\pi}{2}\|f\|_\infty\|A\|_2^2.
\end{aligned}$$

Therefore by Hahn-Banach theorem we conclude that

$$\|\eta_o\|_{L^1([0,2\pi])} = \sup_{f \in L^\infty([0,2\pi]):\|f\|_\infty = 1} \left|\int_0^{2\pi} f(t)\eta_o(t)dt\right| \leq \frac{\pi}{2}\|A\|_2^2.$$

This completes the proof. □

2.3 Reduction to the finite dimension

In this section we prove some estimates similar to those in Section 3 of [22, 63, 41] and use them to reduce the problem in finite dimension. Now we begin with a lemma collecting some results [22, 29, 63, 41] following from the Weyl-von Neumann type construction.

Lemma 2.3.1. *Let U_0 be unitary and let H_0 be self-adjoint operator as in Lemma 1.2.11. Then given a set of normalized vectors $\{f_l\}_{1\leq l\leq L}$ in $\mathcal{H}$ and $\epsilon > 0$ there exist a finite rank projection P such that*

$$(i)\ \ \|P^{\perp}f_l\| < \epsilon \quad for \quad 1\leq l\leq L,$$
$$(ii)\ \ P^{\perp}H_0P \in \mathcal{B}_2(\mathcal{H})\ and\ \|P^{\perp}H_0P\|_2 < \epsilon,$$
$$(iii)\ \ \|P^{\perp}(i\pm H_0)^{-1}P\|_2 < \epsilon,$$
$$(iv)\ \ for\ any\ integer\ m,\ \|P^{\perp}U_0^mP\|_2 < 2|m|\epsilon.$$

Proof. Let $F(\cdot)$ be be the spectral measure associated with the self-adjoint operator H_0. As in the proof of Proposition 3.1 in [22] we set a, $F_k = F(\Delta_k)$, where $\Delta_k = \left(\frac{2k-n-2}{n}a, \frac{2k-n}{n}a\right]$ for $1\leq k\leq n$, and

$$g_{kl} = \begin{cases} \frac{F_kf_l}{\|F_kf_l\|} & \text{if } F_kf_l \neq 0,\\ 0 & \text{if } F_kf_l = 0,\end{cases}$$

for $1\leq k\leq n$ and $1\leq l\leq L$ in such a way so that $\left\|\left[I - F((-a,a])\right]f_l\right\| < \epsilon$ for $1\leq l\leq L$ and $g_{kl}\in F_k\mathcal{H}\subseteq$ Dom(H_0). Let P be the orthogonal projection onto the subspace generated by $\{g_{kl}:\ \ 1\leq k\leq n;\ \ 1\leq l\leq L\}$. Using the Gram-Schmidt orthonormalization process, we can obtain an orthonormal set made out of $\{g_{kl}\}$ which are also in Dom(H_0). So without loss of generality we may assume that $\{g_{kl}\}$ is an orthonormal set.

A simple calculation shows that for $\lambda_k = \frac{2k-n-1}{n}a$,

$$\|\left(H_0-\lambda_k\right)g_{kl}\|^2 = \int_{\frac{2k-n-2}{n}a}^{\frac{2k-n}{n}a}(\lambda-\lambda_k)^2\,\|F(d\lambda)g_{kl}\|^2 \leq \left(\frac{a}{n}\right)^2 \quad \text{for} \quad 1\leq l\leq L,$$

and therefore

$$\|(I-P)H_0Pu\|^2 \leq \left(\frac{a}{n}\right)^2\sum_k\left(\sum_l|\langle u, g_{k,l}\rangle|\right)^2 \leq \frac{a^2}{n^2}\,L\,\|u\|^2 \quad \text{for} \quad u\in\mathcal{H}.$$

The operators $PH_0(I-P)$ and $(I-P)H_0P$ are finite rank operators with rank less than or equal to nL. Hence, using the above estimate we get that

$$\|(I-P)H_0P\|_2 = \|PH_0(I-P)\|_2 \leq \sqrt{dim(P)}\ \|(I-P)H_0P\| \leq \sqrt{nL}\ \left(\frac{a}{n}\right)\ \sqrt{L} = L\ \left(\frac{a}{\sqrt{n}}\right).$$

Therefore by choosing large n, we conclude (i) and (ii).

Next we prove (iii) and (iv). Since F_k commutes with H_0, $(H_0 \pm i)^{-1} g_{_{kl}} = F_k(H_0 \pm i)^{-1} f_l / \|F_k f_l\| \in F_k\mathcal{H}$. Thus by setting $\lambda_k = \frac{2k-n-1}{n} a$ one has

$$\begin{aligned}\|\{(H_0 \pm i)^{-1} - (\lambda_k \pm i)^{-1}\} g_{_{kl}}\|^2 &= \int_{\Delta_k} \left|(\lambda \pm i)^{-1} - (\lambda_k \pm i)^{-1}\right|^2 \|F(d\lambda) g_{_{kl}}\|^2 \\ &\leq \int_{\Delta_k} \left|\lambda - \lambda_k\right|^2 \|F(d\lambda) g_{_{kl}}\|^2 \leq \left(\frac{a}{n}\right)^2.\end{aligned}$$

It is clear that $P^{\perp}(H_0 \pm i)^{-1} g_{_{kl}} \in F_k\mathcal{H}$ and therefore we have for any $u \in \mathcal{H}$

$$\begin{aligned}\|P^{\perp}(H_0 \pm i)^{-1} Pu\|^2 &= \left\|P^{\perp}(H_0 \pm i)^{-1} \sum_{k=1}^{n}\sum_{l=1}^{L} \langle u, g_{_{kl}}\rangle g_{_{kl}}\right\|^2 \\ &= \left\|\sum_{k=1}^{n}\sum_{l=1}^{L} \langle u, g_{_{kl}}\rangle P^{\perp}(H_0 \pm i)^{-1} g_{_{kl}}\right\|^2 \\ &= \sum_{k=1}^{n} \left\|\sum_{l=1}^{L} \langle u, g_{_{kl}}\rangle P^{\perp}(H_0 \pm i)^{-1} g_{_{kl}}\right\|^2 \\ &= \sum_{k=1}^{n} \left\|\sum_{l=1}^{L} \langle u, g_{_{kl}}\rangle P^{\perp}\big((H_0 \pm i)^{-1} - (\lambda_k \pm i)^{-1}\big) g_{_{kl}}\right\|^2 \\ &\leq \sum_{k=1}^{n} \left[\sum_{l=1}^{L} |\langle u, g_{_{kl}}\rangle|\, \left\|P^{\perp}\big((H_0 \pm i)^{-1} - (\lambda_k \pm i)^{-1}\big) g_{_{kl}}\right\|\right]^2 \\ &\leq \left(\frac{a}{n}\right)^2 \sum_{k=1}^{n} \left(\sum_{l=1}^{L} |\langle u, g_{_{kl}}\rangle|\right)^2 \leq \left(\frac{a}{n}\right)^2 L\|u\|^2.\end{aligned}$$

Thus, the Hilbert-Schmidt norm can be estimated to be

$$\|P^{\perp}(H_0 \pm i)^{-1} P\|_2 \leq \sqrt{\dim(P)} \|P^{\perp}(H_0 \pm i)^{-1} P\| \leq \sqrt{nL}\ \left(\frac{a}{n}\right)\sqrt{L} = L\left(\frac{a}{\sqrt{n}}\right). \tag{2.12}$$

Moreover for $m = \pm 1$ the following identity

$$\begin{aligned}P^{\perp} U_0^{\pm 1} P = P^{\perp}\left[e^{\pm i\phi}(i \mp H_0)(i \pm H_0)^{-1}\right] P &= P^{\perp}\left[e^{\pm i\phi}\big\{2i(i \pm H_0)^{-1} - I\big\}\right] P \\ &= 2i\ e^{\pm i\phi} P^{\perp}\left[(i \pm H_0)^{-1}\right] P\end{aligned}$$

along with the above equation (2.12) implies that $\left\|P^{\perp}U_0^{\pm 1}P\right\|_2 \leq 2|\pm 1| L\left(\frac{a}{\sqrt{n}}\right)$ and finally principle of mathematical induction procedure leads to $\left\|P^{\perp}U_0^{m}P\right\|_2 \leq 2|m| L\left(\frac{a}{\sqrt{n}}\right)$ for general m. The proof concludes by choosing n sufficiently large. □

Lemma 2.3.2. *Let U and U_0 be two unitary operators in a separable infinite dimensional Hilbert space $\mathcal{H}$ such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$ and let A be the corresponding self-adjoint operator in $\mathcal{B}_2(\mathcal{H})$ such that $U = e^{iA}U_0$. Then given $\epsilon > 0$, there exists a projection P of finite rank such that for any integer m and for all t with $|t| \leq T$,*

(i) $\|P^{\perp}U_0^{m}P\|_2 < 2|m|\epsilon, \quad \|P^{\perp}A\|_2 < 2\epsilon,$

(ii) $\|P^{\perp}e^{itA}P\|_2 < 2Te^{T\|A\|}\ \epsilon, \quad \|P^{\perp}U^{m}P\|_2 < 2|m|(e^{\|A\|}+1)\ \epsilon.$

Proof. Let $A(\cdot) = \sum_{l=1}^{\infty} \tau_l \langle \cdot, f_l\rangle f_l$ be the canonical form of A with $\sum_{l=1}^{\infty} \tau_l^2 < \infty$. Next choose L in such a way so that $\|A - A_L\|_2 = \sqrt{\sum_{l=L+1}^{\infty} \tau_l^2} < \epsilon$, where $A_L(\cdot) = \sum_{l=1}^{L} \tau_l \langle \cdot, f_l\rangle f_l$ and $\epsilon' = \min\left\{\epsilon, \frac{\epsilon}{\sum_{l=1}^{L}|\tau_l|}\right\} > 0$. Next, we apply Lemma 2.3.1 with H_0 as the correponding self-adjoint operator associated with U_0 (see (1.2)), $\{f_1, f_2, \dots, f_L\}$ and ϵ' in place of ϵ. Hence we get a finite rank projection P in $\mathcal{H}$ such that

$$\|P^{\perp}f_l\| < \epsilon' < \epsilon \quad \text{for} \quad 1 \leq l \leq L \quad \text{and} \quad \|P^{\perp}U_0^{m}P\|_2 < 2|m|\epsilon' < 2|m|\epsilon \quad \text{for any integer } m.$$

Furthermore,

$$\begin{aligned}\|P^{\perp}A\|_2 &\leq \|P^{\perp}(A - A_L)\|_2 + \|P^{\perp}A_L\|_2 \leq \|A - A_L\|_2 + \|P^{\perp}A_L\|_2 \\ &< \epsilon + \left\|\sum_{l=1}^{L} \tau_l \langle \cdot, f_l\rangle P^{\perp}f_l\right\|_2 < \epsilon + \epsilon'\left(\sum_{l=1}^{L}|\tau_l|\right) < 2\epsilon.\end{aligned}$$

For (ii), by the same calculation as in page 831 of [63], it follows that

$$\begin{aligned}\alpha(t) = \|P^{\perp}e^{itA}P\|_2 =& \|P^{\perp}(e^{itA} - I)P\|_2 \\ \leq& \|A\| \int_0^t \alpha(s)\ ds + T\|P^{\perp}AP\|_2 \\ \leq& \|A\| \int_0^t \alpha(s)\ ds + 2T\epsilon \quad \text{for} \quad |t| \leq T \end{aligned} \tag{2.13}$$

solving this Gronwall-type inequality (2.13) leads to

$$\alpha(t) = \|P^{\perp}e^{itA}P\|_2 \leq 2T\epsilon\ e^{t\|A\|} \leq 2Te^{T\|A\|}\epsilon \quad \text{uniformly for t with} \quad |t| \leq T.$$

Moreover by using (i) (for $m = \pm 1$) and (ii) (for $t = \pm 1$) we conclude

$$\|P^\perp UP\|_2 = \|P^\perp e^{iA} U_0 P\|_2 = \|P^\perp e^{iA}(P^\perp + P)U_0 P\|_2 < 2(1 + e^{\|A\|})\,\epsilon$$

and

$$\|P^\perp U^{-1} P\|_2 = \|P^\perp U_0^{-1} e^{-iA} P\|_2 = \|P^\perp U_0^{-1}(P + P^\perp)e^{-iA} P\|_2 < 2(1 + e^{\|A\|})\,\epsilon.$$

Finally mathematical induction procedure leads to $\|P^\perp U^m P\|_2 < 2|m|(e^{\|A\|} + 1)\,\epsilon$ for general m. This completes the proof. □

Lemma 2.3.3. *Let U and U_0 be two unitary operators in a separable infinite dimensional Hilbert space $\mathcal{H}$ such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$ and let A be the corresponding self-adjoint operator in $\mathcal{B}_2(\mathcal{H})$ such that $U = e^{iA}U_0$. Then for $\epsilon > 0$ there exists a finite rank projection P such that for any integers m, k and $|s| \leq T$*

(i) $\|P^\perp\left(e^{iA} - I\right)\|_2 < 2\epsilon, \quad \|\left(e^{isA} - e^{isA_P}\right)P\|_2 < 2T\epsilon,$
$\left\|P^\perp(e^{iA} - iA - I)\right\|_1 < 2\|A\|_2\|A\|^{-2}\,(e^{\|A\|} - \|A\| - 1)\epsilon,$

(ii) $\|\left(U_0^m - U_{0,P}^m\right)P\|_2 < 2|m|\epsilon, \quad \|P\left(U^m - U_P^m\right)P\|_2 < 2|m|\epsilon\left\{(|m| - 1)e^{\|A\|} + (|m| + 1)\right\},$

(iii) $\left|\mathrm{Tr}\left\{PU_P^m\left(e^{iA} - e^{iA_P}\right)U_0^k\right\}\right| < 4\epsilon^2 e^{\|A\|},$

where in the above $U_{0,P} = e^{i\phi}(i - PH_0P)(i + PH_0P)^{-1}$, $U_P = e^{(iPAP)}U_{0,P}$ and $A_P = PAP$.

Remark 2.3.4. *Now observe that P commutes with $(i \pm PH_0P)$, $(i \pm PH_0P)^{-1}$ and PAP and hence P commutes with $U_{0,P}$ and U_P. Thus $PU_{0,P}P$ and PU_PP can be looked upon as unitary operators on the Hilbert space $P\mathcal{H}$*

Proof of Lemma 2.3.3: Given U_0 and A construct H_0 and P as in Lemma 2.3.2 respectively.

(i) First we note that

$$\|P^\perp(e^{iA} - I)\|_2 = \left\|\int_0^1 iP^\perp A e^{isA} ds\right\|_2 \leq \|P^\perp A\|_2 < 2\epsilon,$$

$$\left\|(e^{isA} - e^{isA_P})P\right\|_2 = \left\|\int_0^1 e^{istA} is(A - A_P)Pe^{is(1-t)A_P}dt\right\|_2 \leq T\|P^\perp AP\|_2 < 2T\epsilon,$$

and furthermore

$$\left\|P^{\perp}(e^{iA} - iA - I)\right\|_1 = \left\|P^{\perp}A^2(\sum_{k=2}^{\infty}\frac{(iA)^{k-2}}{k!})\right\|_1$$
$$\leq \|P^{\perp}A\|_2\|A\|_2\left\|\sum_{k=2}^{\infty}\frac{(iA)^{k-2}}{k!}\right\| \leq\ 2\|A\|_2\|A\|^{-2}\ (e^{\|A\|} - \|A\| - 1)\epsilon.$$

(ii) Now we set $U_0^{\#^m} = U_0^{\pm m}$ and $U_{0,P}^{\#^m} = U_{0,P}^{\pm m}$, $m \geq 1$. Thus by using Lemma 2.3.1 (ii), Remark 2.3.4 and the identity

$$\left(U_0^{\#} - U_{0,P}^{\#}\right) P = \mp 2ie^{\pm i\phi}(i \pm H_0)^{-1}\left[P^{\perp}H_0P\right](i \pm PH_0P)^{-1}P$$

we have

$$\left\|(U_0^{\#^m} - U_{0,P}^{\#^m})P\right\|_2 = \left\|\sum_{j=0}^{m-1} U_0^{\#^{m-j-1}}(U_0^{\#} - U_{0,P}^{\#})U_{0,P}^{\#^j}P\right\|_2$$
$$\leq 2\sum_{j=0}^{m-1}\left\|U_0^{\#^{m-j-1}}(i \pm H_0)^{-1}\left[P^{\perp}H_0P\right](i \pm PH_0P)^{-1}U_{0,P}^{\#^j}P\right\|_2$$
$$\leq 2\sum_{j=0}^{m-1}\left\|P^{\perp}H_0P\right\|_2 < 2|m|\epsilon.$$

Now first we note that

$$\begin{aligned}\|P(U - U_P)P\|_2 =&\ \left\|P(e^{iA}U_0 - e^{PAP}U_{0,P})P\right\|_2\\ \leq&\ \left\|Pe^{iA}(U_0 - U_{0,P})P\right\|_2 + \left\|P(e^{iA} - e^{iA_P})U_{0,P}P\right\|_2\\ \leq&\ \left\|(U_0 - U_{0,P})P\right\|_2 + \left\|P(e^{iA} - e^{iA_P})\right\|_2 <\ 4\epsilon,\end{aligned} \tag{2.14}$$

by using (i), (ii). Furthermore, since P commutes with U_P, we have for $m \geq 1$

$$\left\|P(U^m - U_P^m)P\right\|_2 = \left\|\sum_{j=0}^{m-1} PU^{m-j-1}(U - U_P)U_P^jP\right\|_2$$
$$\leq \sum_{j=0}^{m-1}\left\{\left\|PU^{m-j-1}P^{\perp}(U - U_P)U_P^jP\right\|_2 + \left\|PU^{m-j-1}P(U - U_P)PU_P^jP\right\|_2\right\}$$
$$\leq \sum_{j=0}^{m-1}\left\{2\left\|PU^{m-j-1}P^{\perp}\right\|_2 + \left\|P(U - U_P)P\right\|_2\right\} <\ 2m\epsilon\left\{(m-1)e^{\|A\|} + (m+1)\right\},$$

by using the above equation 2.14 and Lemma 2.3.2 (ii). Finally the estimate for $m \leq -1$ follows by taking the adjoint.

(*iii*) Now by applying trace properties and using Lemma 2.3.2 (*i*), (*ii*) we conclude that

$$\begin{aligned}
&\left|\operatorname{Tr}\left\{PU_P^m(e^{iA}-e^{iA_P})U_0^k\right\}\right| \\
&= \left|\operatorname{Tr}\left[PU_P^m\left(\int_0^1\left\{e^{isA}i(A-A_P)Pe^{i(1-s)A_P}\right\}ds\right)\ U_0^k\right]\right| \\
&= \left|\int_0^1 \operatorname{Tr}\left[PU_p^m e^{isA}P^{\perp}APe^{i(1-s)A_P}U_0^k\right]\,ds\right| \\
&= \left|\int_0^1 \operatorname{Tr}\left[P^{\perp}AP\ e^{i(1-s)A_P}U_0^kPU_P^m\ Pe^{isA}P^{\perp}\right]\,ds\right| \\
&\leq \int_0^1 \|P^{\perp}AP\|_2\left\|Pe^{isA}P^{\perp}\right\|_2 ds <\ 4\epsilon^2 e^{\|A\|}.
\end{aligned}$$

Remark 2.3.5. *We can reformulate the above set of lemmas by saying that there exists a sequence* $\{P_n\}$ *of finite rank projections such that for* $m,k\in\mathbb{Z}$ *and* $|s|\leq T$*,*

(*i*) $\|P_n^{\perp}H_0P_n\|_2,\ \ \|P_n^{\perp}U_0^mP_n\|_2,\ \ \|P_n^{\perp}U^mP_n\|_2,\ \ \|P_n^{\perp}A\|_2\ \longrightarrow 0$ *as* $n\longrightarrow\infty$,

(*ii*) $\left\|P_n^{\perp}(e^{iA}-I)\right\|_2,\ \ \left\|(U_0^m-U_{0,n}^m)P_n\right\|_2,\ \ \left\|P_n(U^m-U_n^m)P_n\right\|_2\ \longrightarrow 0$ *as* $n\longrightarrow\infty$,

(*iii*) $\left\|(e^{isA}-e^{isA_{P_n}})P_n\right\|_2,\ \ \left\|P_n^{\perp}e^{isA}P_n\right\|_2,\ \ \left|\operatorname{Tr}\left\{P_nU_n^m\left(e^{iA}-e^{iA_{P_n}}\right)U_0^k\right\}\right|\to 0$ *as* $n\to\infty$,

(*iv*) $\left\|P_n^{\perp}(e^{iA}-iA-I)\right\|_1\longrightarrow 0$ *as* $n\longrightarrow\infty$,

where $A_n=P_nAP_n$, $U_{0,n}=e^{i\phi}(i-P_nH_0P_n)(i+P_nH_0P_n)^{-1}$, $U_n=e^{(iA_n)}U_{0,n}$ *and* $U_{s,n}=e^{(isA_n)}U_{0,n}$.

The next theorem show how the above set of lemmas can be used to reduce the relevant problem into a finite dimensional one.

Theorem 2.3.6. *Let* U *and* U_0 *be two unitary operators in a separable Hilbert space* $\mathcal{H}$ *such that* $U-U_0\in\mathcal{B}_2(\mathcal{H})$ *and let* $A\in\mathcal{B}_2(\mathcal{H})$ *be the corresponding self-adjoint operator as in Theorem 2.2.1 such that* $U=e^{iA}U_0$*. Let* $U_s=e^{isA}U_0,\ s\in\mathbb{R}$ *and* $p(\cdot)$ *be any trigonometric polynomial on* $\mathbb{T}$ *with complex coefficients. Then there exists a sequence* $\{P_n\}$ *of finite rank projections in* $\mathcal{H}$ *such that*

$$\begin{aligned}
&\operatorname{Tr}\left\{p(U)-p(U_0)-\frac{d}{ds}\bigg|_{s=0}p(U_s)\right\} \\
&\qquad= \lim_{n\to\infty}\operatorname{Tr}\ \left[P_n\left\{p(U_n)-p(U_{0,n})-\frac{d}{ds}\bigg|_{s=0}p(U_{s,n})\right\}P_n\right], \qquad (2.15)
\end{aligned}$$

where $A_n = P_nAP_n$, $U_{0,n} = e^{i\phi}(i - P_nH_0P_n)(i + P_nH_0P_n)^{-1}$, $U_n = e^{(iA_n)}U_{0,n}$ *and* $U_{s,n} = e^{(isA_n)}U_{0,n}$.

Proof. It will be sufficient to prove the theorem for $p(\lambda) = \lambda^r, r \in \mathbb{Z}, \lambda \in \mathbb{T}$. Note that for $r = 0$, both sides of (2.15) are identically zero. First we prove for $r \geq 1$. Using the sequence $\{P_n\}$ of finite rank projections as obtained in Lemma 2.3.2 and Lemma 2.3.3 and using an expression similar to (2.5) in $\mathcal{B}(\mathcal{H})$, we have that

$$
\begin{aligned}
&\operatorname{Tr}\left\{\left[p(U) - p(U_0) - \frac{d}{ds}\bigg|_{s=0} p(U_s)\right] - P_n\left[p(U_n) - p(U_{0,n}) - \frac{d}{ds}\bigg|_{s=0} p(U_{s,n})\right]P_n\right\} \\
&= \operatorname{Tr}\left\{\left[U^r - U_0^r - \sum_{j=0}^{r-1} U_0^{r-j-1}(iA)U_0^{j+1}\right] - P_n\left[U_n^r - U_{0,n}^r - \sum_{j=0}^{r-1} U_{0,n}^{r-j-1}(iA_n)U_{0,n}^{j+1}\right]P_n\right\} \\
&= \operatorname{Tr}\left\{\left[\sum_{j=0}^{r-1} U^{r-j-1}(U - U_0)U_0^j - \sum_{j=0}^{r-1} U_0^{r-j-1}(iA)U_0^{j+1}\right]\right. \\
&\qquad\qquad \left. - P_n\left[\sum_{j=0}^{r-1} U_n^{r-j-1}P_n(U_n - U_{0,n})P_nU_{0,n}^j - \sum_{j=0}^{r-1} U_{0,n}^{r-j-1}(iA_n)U_{0,n}^{j+1}\right]P_n\right\} \\
&= \operatorname{Tr}\left\{\left[\sum_{j=0}^{r-1} U^{r-j-1}(e^{iA} - I)U_0^{j+1} - \sum_{j=0}^{r-1} U_0^{r-j-1}(iA)U_0^{j+1}\right]\right. \\
&\qquad\qquad \left. - P_n\left[\sum_{j=0}^{r-1} U_n^{r-j-1}P_n(e^{iA_n} - I)P_nU_{0,n}^{j+1} - \sum_{j=0}^{r-1} U_{0,n}^{r-j-1}(iA_n)U_{0,n}^{j+1}\right]P_n\right\} \\
&= \operatorname{Tr}\left\{\sum_{j=0}^{r-1}\left[U^{r-j-1}(e^{iA} - iA - I)U_0^{j+1} + (U^{r-j-1} - U_0^{r-j-1})(iA)U_0^{j+1}\right]\right. \\
&\left. - P_n\left(\sum_{j=0}^{r-1}\left[U_n^{r-j-1}P_n(e^{iA_n} - iA_n - I)P_nU_{0,n}^{j+1} + (U_n^{r-j-1} - U_{0,n}^{r-j-1})(iA_n)U_{0,n}^{j+1}\right]\right)P_n\right\} \\
&= \operatorname{Tr}\left\{\sum_{j=0}^{r-1}\left[U^{r-j-1}(e^{iA} - iA - I)U_0^{j+1} - P_nU_n^{r-j-1}P_n(e^{iA_n} - iA_n - I)P_nU_{0,n}^{j+1}P_n\right]\right. \\
&\quad \left. + \sum_{j=0}^{r-1}\left[(U^{r-j-1} - U_0^{r-j-1})(iA)U_0^{j+1} - P_n(U_n^{r-j-1} - U_{0,n}^{r-j-1})P_n(iA_n)U_{0,n}^{j+1}P_n\right]\right\}.
\end{aligned}
\tag{2.16}
$$

Using the results obtained in Lemma 2.3.2 and Lemma 2.3.3, the first term of the expression (2.16) leads to

$$
\left|\operatorname{Tr}\left\{\sum_{j=0}^{r-1}\left[U^{r-j-1}(e^{iA} - iA - I)U_0^{j+1} - P_nU_n^{r-j-1}P_n(e^{iA_n} - iA_n - I)P_nU_{0,n}^{j+1}P_n\right]\right\}\right|
$$

$$
\begin{aligned}
&= \Bigg| \operatorname{Tr}\Bigg\{ \sum_{j=0}^{r-1} \Big[(U^{r-j-1} - U_n^{r-j-1}) P_n (e^{iA} - iA - I) U_0^{j+1} + U^{r-j-1} P_n^{\perp} (e^{iA} - iA - I) U_0^{j+1} \\
&\qquad + U_n^{r-j-1} P_n (e^{iA} - iA - I - e^{iA_n} + iA_n + I) U_0^{j+1} \\
&\qquad + U_n^{r-j-1} P_n (e^{iA_n} - iA_n - I) P_n (U_0^{j+1} - U_{0,n}^{j+1}) \Big] \Bigg\} \Bigg| \\
&= \Bigg| \operatorname{Tr}\Bigg\{ \sum_{j=0}^{r-1} \Big[P_n (U^{r-j-1} - U_n^{r-j-1}) P_n (e^{iA} - iA - I) U_0^{j+1} + P_n^{\perp} U^{r-j-1} P_n (e^{iA} - iA - I) U_0^{j+1} \\
&\qquad + U^{r-j-1} P_n^{\perp} (e^{iA} - iA - I) U_0^{j+1} + U_n^{r-j-1} P_n (e^{iA} - iA - e^{iA_n} + iA_n +) U_0^{j+1} \\
&\qquad + U_n^{r-j-1} P_n (e^{iA_n} - iA_n - I) P_n (U_0^{j+1} - U_{0,n}^{j+1}) \Big] \Bigg\} \Bigg| \\
&\le \sum_{j=0}^{r-1} \Big\{ \big\| P_n (U^{r-j-1} - U_n^{r-j-1}) P_n \big\|_2 \, \big\| (e^{iA} - iA - I) \big\|_2 + \big\| P_n^{\perp} U^{r-j-1} P_n \big\|_2 \, \big\| e^{iA} - iA - I \big\|_2 \\
&\qquad + \big\| P_n^{\perp} (e^{iA} - iA - I) \big\|_1 + \Big| \operatorname{Tr}\big(P_n U_n^{r-j-1} P_n (e^{iA} - iA - e^{iA_n} + iA_n) U_0^{j+1} P_n \big) \Big| \\
&\qquad + \big\| (e^{iA_n} - iA_n - I) \big\|_2 \big\| P_n (U_0^{j+1} - U_{0,n}^{j+1}) \big\|_2 \Big\} \\
&\le \big(e^{\|A\|} - \|A\| - 1 \big) \|A\|^{-1} \sum_{j=0}^{r-1} \Big\{ \big\| P_n (U^{r-j-1} - U_n^{r-j-1}) P_n \big\|_2 + \big\| P_n^{\perp} U^{r-j-1} P_n \big\|_2 \Big\} \\
&\quad + r \big\| P_n^{\perp} (e^{iA} - iA - I) \big\|_1 + \sum_{j=0}^{r-1} \Big| \operatorname{Tr}\big(P_n U_n^{r-j-1} P_n (e^{iA} - e^{iA_n}) U_0^{j+1} P_n \big) \Big| \\
&\quad + \sum_{j=0}^{r-1} \big\| P_n U_n^{r-j-1} P_n A P_n^{\perp} U_0^{j+1} P_n \big\|_1 + \big(e^{\|A\|} - \|A\| - 1 \big) \|A\|^{-1} \sum_{j=0}^{r-1} \big\| P_n (U_0^{j+1} - U_{0,n}^{j+1}) \big\|_2 \\
&\le \big(e^{\|A\|} - \|A\| - 1 \big) \|A\|^{-1} \sum_{j=0}^{r-1} \Big\{ \big\| P_n (U^{r-j-1} - U_n^{r-j-1}) P_n \big\|_2 + \big\| P_n^{\perp} U^{r-j-1} P_n \big\|_2 \\
&\qquad + \big\| P_n (U_0^{j+1} - U_{0,n}^{j+1}) \big\|_2 \Big\} + r \big\| P_n^{\perp} (e^{iA} - iA - I) \big\|_1 \\
&\quad + \sum_{j=0}^{r-1} \Big| \operatorname{Tr}\big(P_n U_n^{r-j-1} P_n (e^{iA} - e^{iA_n}) U_0^{j+1} P_n \big) \Big| + \big\| P_n A P_n^{\perp} \big\|_2 \sum_{j=0}^{r-1} \big\| P_n^{\perp} U_0^{j+1} P_n \big\|_2,
\end{aligned} \tag{2.17}
$$

and the estimate of the second term of the right hand side of (2.16) is as follows

$$
\begin{aligned}
&\Bigg| \operatorname{Tr}\Bigg(\sum_{j=0}^{r-1} \Big[(U^{r-j-1} - U_0^{r-j-1}) A U_0^{j+1} - P_n (U_n^{r-j-1} - U_{0,n}^{r-j-1}) P_n A_n U_{0,n}^{j+1} \Big] \Bigg) \Bigg| \\
=& \Bigg| \operatorname{Tr}\Bigg(\sum_{j=0}^{r-1} \Big[\big\{ (U^{r-j-1} - U_0^{r-j-1}) - (U_n^{r-j-1} - U_{0,n}^{r-j-1}) \big\} P_n A U_0^{j+1} \\
&\quad + (U^{r-j-1} - U_0^{r-j-1}) P_n^{\perp} A U_0^{j+1} + (U_n^{r-j-1} - U_{0,n}^{r-j-1}) P_n (A - A_n) U_0^{j+1}
\end{aligned}
$$

$$+ (U_n^{r-j-1} - U_{0,n}^{r-j-1})P_n A_n P_n (U_0^{j+1} - U_{0,n}^{j+1})\Big]\Big)\Big|$$

$$\leq \sum_{j=0}^{r-1} \Big\{ \Big(\big\|(U^{r-j-1} - U_n^{r-j-1})P_n\big\|_2 + \big\|(U_0^{r-j-1} - U_{0,n}^{r-j-1})P_n\big\|_2 \Big) \big\|P_n A U_0^{j+1}\big\|_2$$

$$+ \big\|U^{r-j-1} - U_0^{r-j-1}\big\|_2 \big\|P_n^{\perp} A U_0^{j+1}\big\|_2 + \big\|(U_n^{r-j-1} - U_{0,n}^{r-j-1})P_n\big\|_2 \big\|P_n A P_n^{\perp}\big\|_2$$

$$+ 2\|A\|_2 \big\|P_n (U_0^{j+1} - U_{0,n}^{j+1})\big\|_2 \Big\}$$

$$\leq \|A\|_2 \sum_{j=0}^{r-1} \Big\{ \big\|(U^{r-j-1} - U_n^{r-j-1})P_n\big\|_2 + \big\|(U_0^{r-j-1} - U_{0,n}^{r-j-1})P_n\big\|_2$$

$$+ 2\big\|P_n (U_0^{j+1} - U_{0,n}^{j+1})\big\|_2 \Big\} + \frac{r(r-1)}{2} \|A\|_2 \big\|P_n^{\perp} A\big\|_2. \tag{2.18}$$

Now using all estimates listed in Remark (2.3.5) we conclude that the right hand sides of (2.17) and (2.18) tend to zero as n approaches to infinity. Hence from (2.16) we deduce the desire approximation (2.15). On the other hand for $p(\lambda) = \lambda^r$, $r \leq -1$, we have

$$\mathrm{Tr}\Big\{ \Big[p(U) - p(U_0) - \frac{d}{ds}\Big|_{s=0} p(U_s) \Big] - P_n \Big[p(U_n) - p(U_{0,n}) - \frac{d}{ds}\Big|_{s=0} p(U_{s,n}) \Big] P_n \Big\}$$

$$= \mathrm{Tr}\Big\{ \sum_{j=0}^{|r|-1} \Big(U^{*|r|-j-1} U_0^* (e^{-iA} - 1) U_0^{*j} + U_0^{*|r|-j-1} U_0^* (iA) U_0^{*j} \Big)$$

$$- P_n \sum_{j=0}^{|r|-1} \Big(U_n^{*|r|-j-1} U_{0,n}^* (e^{-iA_n} - 1) {U_{0,n}^*}^{j} + {U_{0,n}^*}^{|r|-j-1} U_{0,n}^* (iA_n) {U_{0,n}^*}^{j} \Big) P_n \Big\}$$

$$= \mathrm{Tr}\Big\{ \sum_{j=0}^{|r|-1} \Big[U^{*|r|-j-1} U_0^* (e^{-iA} + iA - I) U_0^{*j}$$

$$- P_n U_n^{*|r|-j-1} U_{0,n}^* P_n (e^{-iA_n} + iA_n - I) P_n {U_{0,n}^*}^{j} P_n \Big] - \sum_{j=0}^{|r|-1} \Big[(U^{*|r|-j-1} - U_0^{*|r|-j-1}) U_0^* (iA) U_0^{*j}$$

$$- P_n (U_n^{*|r|-j-1} - {U_{0,n}^*}^{|r|-j-1}) U_{0,n}^* P_n (iA_n) {U_{0,n}^*}^{j} P_n \Big] \Big\}. \tag{2.19}$$

Similarly as above with an appropriate rearrangement and using Remark 2.3.5, one can show that the right-hand side of (2.19) approaches to zero as n tends to infinity. This completes the proof. □

2.4 Existence of shift function

In this section, we derive the trace formula corresponding to the pair (U, U_0). The following theorem is one of the main result in this section.

Theorem 2.4.1. *Let U and U_0 be two unitary operators in a separable Hilbert space $\mathcal{H}$ such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$ and let $A \in \mathcal{B}_2(\mathcal{H})$ be the corresponding self-adjoint operator as in Theorem 2.2.1 such that $U = e^{iA}U_0$. Denote $U_s = e^{isA}U_0$, $s \in \mathbb{R}$. Then for any trigonometric polynomial $p(\cdot)$ on $\mathbb{T}$ with complex coefficients,*

$$\left\{p(U) - p(U_0) - \frac{d}{ds}p(U_s)\Big|_{s=0}\right\} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists an $L^1([0, 2\pi])$- function η (unique upto an additive constant) such that

$$\operatorname{Tr}\left\{p(U) - p(U_0) - \frac{d}{ds}p(U_s)\Big|_{s=0}\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\{p(e^{it})\}\eta(t)dt.$$

Moreover, $\|\eta\|_{L^1([0,2\pi])} \leq \frac{\pi}{2}\|A\|_2^2$.

Proof. By Theorems 2.2.2 and 2.3.6, we have that

$$\begin{aligned}
&\operatorname{Tr}\left\{p(U) - p(U_0) - \frac{d}{ds}p(U_s)\Big|_{s=0}\right\}\\
&= \lim_{n\to\infty} \operatorname{Tr}\left[P_n\left\{p(U_n) - p(U_{0,n}) - \frac{d}{ds}\Big|_{s=0} p(U_{s,n})\right\}P_n\right]\\
&= \lim_{n\to\infty} \int_0^{2\pi} \frac{d^2}{dt^2}\{p(e^{it})\}\eta_n(t)dt = \lim_{n\to\infty} \int_0^{2\pi} \frac{d^2}{dt^2}\{p(e^{it})\}\eta_{o,n}(t)dt,
\end{aligned}$$

where

$$\eta_{o,n}(t) = \eta_n(t) - \frac{1}{2\pi}\int_0^{2\pi} \eta_n(s)ds\ ,\quad t \in [0, 2\pi] \quad \text{and} \quad \|\eta_{o,n}\|_{L^1([0,2\pi])} \leq \frac{\pi}{2}\|A\|_2^2. \tag{2.20}$$

Next we want to show that $\{\eta_{o,n}\}$ is a Cauchy sequence in $L^1([0, 2\pi])$. Indeed, for any $f \in L^\infty([0, 2\pi])$ we consider

$$f_o(t) = f(t) - \frac{1}{2\pi}\int_0^{2\pi} f(s)ds.$$

Now it is easy to observe that

$$\int_0^{2\pi} f(t)\{\eta_{o,n}(t) - \eta_{o,m}(t)\}dt = \int_0^{2\pi} f_o(t)\{\eta_n(t) - \eta_m(t)\}dt,$$

$$\int_0^{2\pi} f_o(t)dt = 0 \quad \text{and } \|f_o\|_\infty \leq 2\|f\|_\infty.$$

Therefore by following the idea contained in the paper of Gesztesy et al.[26] (see also [22]), using the expression (2.7) of η, using Fubini's theorem to interchange the orders of integration and integrating by-parts, we have for $g(e^{it}) = \int\limits_0^t f_o(s)ds,\ t \in [0, 2\pi]$ that

$$\begin{aligned}
&\int_0^{2\pi} f(t)\big\{\eta_{o,n}(t) - \eta_{o,m}(t)\big\}dt = \int_0^{2\pi} f_o(t)\big\{\eta_n(t) - \eta_m(t)\big\}dt \\
&= \int_0^{2\pi} \frac{d}{dt}\{g(e^{it})\}\left(\int_0^1 \mathrm{Tr}\left[A_n\big\{E_{0,n}(t) - E_{s,n}(t)\big\} - A_m\big\{E_{0,m}(t) - E_{s,m}(t)\big\}\right] ds\right) dt \\
&= \int_0^1 ds \int_0^{2\pi} \frac{d}{dt}\big\{g(e^{it})\big\}\ \mathrm{Tr}\left[A_n\big\{E_{0,n}(t) - E_{s,n}(t)\big\} - A_m\big\{E_{0,m}(t) - E_{s,m}(t)\big\}\right]dt \\
&= \int_0^1 ds \left(g(e^{it})\ \mathrm{Tr}\left[A_n\big\{E_{0,n}(t) - E_{s,n}(t)\big\} - A_m\big\{E_{0,m}(t) - E_{s,m}(t)\big\}\right]\Bigg|_{t=0}^{2\pi} \right. \\
&\qquad \left. - \int_0^{2\pi} g(e^{it})\ \mathrm{Tr}\left[A_n\big\{E_{0,n}(dt) - E_{s,n}(dt)\big\} - A_m\big\{E_{0,m}(dt) - E_{s,m}(dt)\big\}\right]\right) \\
&= -\int_0^1 ds \int_0^{2\pi} g(e^{it})\ \mathrm{Tr}\left[A_n\big\{E_{0,n}(dt) - E_{s,n}(dt)\big\} - A_m\big\{E_{0,m}(dt) - E_{s,m}(dt)\big\}\right] \\
&= \int_0^1 ds\ \mathrm{Tr}\left[A_n\big\{g(U_{s,n}) - g(U_{0,n})\big\} - A_m\big\{g(U_{s,m}) - g(U_{0,m})\big\}\right] \\
&= \int_0^1 ds\ \mathrm{Tr}\left[A_n\Big\{\big\{g(U_{s,n}) - g(U_s)\big\} - \big\{g(U_{0,n}) - g(U_0)\big\}\Big\}\right. \\
&\quad \left. - A_m\Big\{\big\{g(U_{s,m}) - g(U_s)\big\} - \big\{g(U_{0,m}) - g(U_0)\big\}\Big\} + (A_n - A_m)\big\{g(U_s) - g(U_0)\big\}\right],
\end{aligned}$$

where $E_{s,n}(\cdot)$ and $E_{0,n}(\cdot)$ are the spectral measures determined uniquely by the unitary operators $U_{s,n}$ and $U_{0,n}$ respectively such that they are continuous at $t = 0$ and noted that all the boundary terms vanishes. Next we note that as in (2.10)

$$P_n\big\{g(U_{s,n}) - g(U_s)\big\}P_n = P_n\left\{\int_0^{2\pi}\int_0^{2\pi} \frac{g(e^{i\lambda}) - g(e^{i\mu})}{e^{i\lambda} - e^{i\mu}}\ \mathcal{G}_n(d\lambda \times d\mu)\Big(P_n\big\{U_{s,n} - U_s\big\}\Big)\right\}P_n,$$

where $\mathcal{G}_n(\Delta \times \delta)(V) = E_{s,n}(\Delta)VE_s(\delta)$ ($V \in \mathcal{B}_2(\mathcal{H}),\ \ \Delta \times \delta \subseteq \mathbb{R} \times \mathbb{R}$ and $E_s(\cdot)$ is the spectral measure determined uniquely by the unitary operator U_s such that it is continuous at 0) extends to a spectral measure on $\mathbb{R}^2$ in the Hilbert space $\mathcal{B}_2(\mathcal{H})$ (equipped with the inner product derived from the trace) and its total variation is less than or equal to $\|V\|_2$. Therefore

$$\big\|P_n\{g(U_{s,n}) - g(U_s)\}P_n\big\|_2 \leq \pi\|f\|_\infty\|P_n\{U_{s,n} - U_s\}\|_2,$$

since $\left|\frac{g(e^{i\lambda})-g(e^{i\mu})}{e^{i\lambda}-e^{i\mu}}\right| \leq \frac{\pi}{2}\|f_o\|_\infty \leq \pi\|f\|_\infty$, for $\lambda,\mu\in[0,2\pi]$. But on the other hand

$$\begin{aligned}
&\big\|P_n(U_{s,n}-U_s)\big\|_2 \leq \big\|P_n(e^{isA_n}-e^{isA})U_{0,n}+P_ne^{isA}(U_{0,n}-U_0)\big\|_2\\
&\leq \big\|P_n(e^{isA_n}-e^{isA})\big\|_2+\big\|P_ne^{isA}P_n(U_{0,n}-U_0)\big\|_2+\big\|P_ne^{isA}P_n^\perp(U_{0,n}-U_0)\big\|_2\\
&\leq \big\|P_n(e^{isA_n}-e^{isA})\big\|_2+\big\|P_n(U_{0,n}-U_0)\big\|_2+2\big\|P_ne^{isA}P_n^\perp\big\|_2\\
&\leq \big\|P_nAP_n^\perp\big\|_2+\big\|P_n(U_{0,n}-U_0)\big\|_2+2s\big\|AP_n^\perp\big\|_2,
\end{aligned}$$

and hence

$$\left|\operatorname{Tr}\Big[A_n\{g(U_{s,n})-g(U_s)\}\Big]\right| \leq \pi\|f\|_\infty\|A\|_2\Big\{\big\|P_nAP_n^\perp\big\|_2+\big\|P_n(U_{0,n}-U_0)\big\|_2+2s\big\|AP_n^\perp\big\|_2\Big\}. \tag{2.21}$$

Similarly we conclude that

$$\left|\operatorname{Tr}\Big[A_n\{g(U_{0,n})-g(U_0)\}\Big]\right| \leq \pi\|f\|_\infty\|A\|_2\ \|P_n(U_{0,n}-U_0)\|_2. \tag{2.22}$$

Furthermore, we also have

$$\begin{aligned}
\left|\operatorname{Tr}\Big[(A_n-A_m)\{g(U_s)-g(U_0)\}\Big]\right| &\leq \pi\|f\|_\infty\ \|A_n-A_m\|_2\ \|U_s-U_0\|_2\\
&\leq \pi\|f\|_\infty\ \|A_n-A_m\|_2\ (s\|A\|_2),
\end{aligned} \tag{2.23}$$

by using the estimate as in (2.11). Therefore using equations (2.21),(2.22) and (2.23) we get

$$\begin{aligned}
&\left|\int_0^{2\pi} f(t)\{\eta_{o,n}(t)-\eta_{o,m}(t)\}dt\right|\\
&\leq \int_0^1 ds\ \Bigg|\operatorname{Tr}\Bigg[A_n\Big\{\{g(U_{s,n})-g(U_s)\}-\{g(U_{0,n})-g(U_0)\}\Big\}\\
&\quad -A_m\Big\{\{g(U_{s,m})-g(U_s)\}-\{g(U_{0,m})-g(U_0)\}\Big\}+(A_n-A_m)\{g(U_s)-g(U_0)\}\Bigg]\Bigg|\\
&\leq K_{m,n}\|f\|_\infty,
\end{aligned}$$

where

$$\begin{aligned}
K_{m,n}=&\pi\|A\|_2\Bigg[\ \Big\{\big\|P_nAP_n^\perp\big\|_2+\big\|P_n(U_{0,n}-U_0)\big\|_2+\big\|AP_n^\perp\big\|_2+\|P_n(U_{0,n}-U_0)\|_2\Big\}\\
&+\ \Big\{\big\|P_mAP_m^\perp\big\|_2+\big\|P_m(U_{0,m}-U_0)\big\|_2+\big\|AP_m^\perp\big\|_2+\|P_m(U_{0,m}-U_0)\|_2\Big\}\\
&+\frac{1}{2}\ \|A_n-A_m\|_2\Bigg].
\end{aligned}$$

Therefore by the Hahn-Banach theorem

$$\|\eta_{o,n} - \eta_{o,m}\|_1 = \sup_{f\in L^\infty([0,2\pi]):\|f\|_\infty=1} \left| \int_0^{2\pi} f(t)\big\{\eta_{o,n}(t) - \eta_{o,m}(t)\big\}dt \right| \leq K_{m,n} \to 0 \text{ as } m,n\to\infty,$$

by using Remark 2.3.5 and hence $\{\eta_{o,n}\}$ is a Cauchy sequence in $L^1([0,2\pi])$. Therefore there exists a $\eta \in L^1([0,2\pi])$ such that $\eta_{o,n}$ converges to η in $L^1([0,2\pi])$ norm. Thus

$$\begin{aligned} &\operatorname{Tr}\left\{p(U) - p(U_0) - \frac{d}{ds}p(U_s)\Big|_{s=0}\right\} \\ &= \lim_{n\to\infty}\int_0^{2\pi} \frac{d^2}{dt^2}\big\{p(e^{it})\big\}\eta_{o,n}(t)dt = \int_0^{2\pi} \frac{d^2}{dt^2}\big\{p(e^{it})\big\}\eta(t)dt. \end{aligned} \tag{2.24}$$

Moreover, from (2.20) it follows that $\|\eta\|_{L^1([0,2\pi])} \leq \frac{\pi}{2}\|A\|_2^2$. Regarding uniqueness of η, let η_1 and η_2 be two $L^1([0,2\pi])$ functions which satisfy (2.24) for any polynomial $p(\cdot)$ on $\mathbb{T}$. Now by considering $p(z) = z^n$ for $n \in \mathbb{Z}\setminus\{0\}$ we get

$$\int_0^{2\pi} e^{int}\,\big\{\eta_1(t) - \eta_2(t)\big\}dt = 0 \qquad \forall n \in \mathbb{Z}\setminus\{0\},$$

and consequently uniqueness of Fourier series implies $(\eta_1 - \eta_2)$ is constant. This completes the proof. □

Our next aim is to extend the class of functions ϕ for which the trace formula (2.4) hold true.

Lemma 2.4.2. *Let $f_n(s) = a_nU_s^n$, where $a_n \in \mathbb{C}$ and $U_s = e^{isA}U_0$ as in the statement of Theorem 2.4.1 be such that $\sum_{n=-\infty}^{\infty} n^2|a_n| < \infty$. Then*

$$\frac{d}{ds}\Big|_{s=0}\left(\sum_{n=-\infty}^{\infty} f_n(s)\right) = \sum_{n=-\infty}^{\infty}\left(\frac{d}{ds}\Big|_{s=0} f_n(s)\right), \tag{2.25}$$

where the infinite series on both sides of (2.25) converge in operator norm.

Proof. The expression in (2.5) along with the fact $\sum_{n=0}^{\infty} n^2|a_n| < \infty$ implies both infinite series in (2.25) converge in operator norm. Next we denote $\tau_n = \operatorname{sgn}(n), n \in \mathbb{Z}$. Then the definition of Gâteaux derivative and the following estimate

$$\left\| \frac{1}{s}\left[\sum_{n=-\infty}^{\infty} a_nU_s^{\tau_n|n|} - \sum_{n=-\infty}^{\infty} a_nU_0^{\tau_n|n|}\right] - \sum_{n=-\infty}^{\infty} a_n \begin{cases} \sum\limits_{j=0}^{|n|-1} U_0^{|n|-j-1}\,(iA)\,U_s^{j+1} & \text{if } n \geq 1, \\ 0 & \text{if } n = 0, \\ -\sum\limits_{j=0}^{|n|-1} (U_0^*)^{|n|-j}\,(iA)\,(U_0^*)^j & \text{if } n \leq -1, \end{cases} \right\|$$

$$\leq \left\{ \sum_{n=1}^{\infty} \left(\left\{ |a_n| + |a_{-n}| \right\} \cdot \left[\frac{n(n-1)}{2} \|A\|^2 + n \left(e^{\|A\|} - \|A\| - 1 \right) \right] \right) \right\} \cdot |s| \quad \longrightarrow 0 \text{ as } s \longrightarrow 0,$$

yields equation (2.25). □

Theorem 2.4.3. *Let U and U_0 be two unitary operators in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$. Then for any $\Phi \in \mathcal{F}_2(\mathbb{T})$,*

$$\left\{ \Phi(U) - \Phi(U_0) - \frac{d}{ds}\Phi(U_s)\Big|_{s=0} \right\} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists an $L^1([0, 2\pi])$- function η, unique up to an additive constant, such that

$$\operatorname{Tr}\left\{ \Phi(U) - \Phi(U_0) - \frac{d}{ds}\Big|_{s=0} \Phi(U_s) \right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\{\Phi(e^{it})\}\eta(t)dt.$$

Proof. Using the above Lemma 2.4.2 we have

$$\begin{aligned}
\Phi(U) - \Phi(U_0) - \frac{d}{ds}\Big|_{s=0} \Phi(U_s) &= \sum_{n=-\infty}^{\infty} a_n U^{\tau_n|n|} - \sum_{n=-\infty}^{\infty} a_n U_0^{\tau_n|n|} - \frac{d}{ds}\Big|_{s=0} \left(\sum_{n=-\infty}^{\infty} a_n U_s^{\tau_n|n|} \right) \\
&= \sum_{n=-\infty}^{\infty} a_n \left[U^{\tau_n|n|} - U_0^{\tau_n|n|} - \frac{d}{ds}\Big|_{s=0} U_s^{\tau_n|n|} \right].
\end{aligned} \tag{2.26}$$

Moreover, using (2.5) we conclude that $\left(U^{\tau_n|n|} - U_0^{\tau_n|n|} - \frac{d}{ds}\Big|_{s=0} U_s^{\tau_n|n|} \right)$ is trace class and the following trace norm estimate

$$\begin{aligned}
&\left\| U^{\tau_n|n|} - U_0^{\tau_n|n|} - \frac{d}{ds}\Big|_{s=0} U_s^{\tau_n|n|} \right\|_1 \\
&= \left\| U^{\tau_n|n|} - U_0^{\tau_n|n|} - \begin{cases} \sum_{j=0}^{|n|-1} U_0^{|n|-j-1}\ (iA)\ U_s^{j+1} & \text{if } n \geq 1, \\ 0 & \text{if } n = 0, \\ -\sum_{j=0}^{|n|-1} (U_0^*)^{|n|-j}\ (iA)\ (U_0^*)^j & \text{if } n \leq -1 \end{cases} \right\|_1 \\
&\leq \left[\frac{|n|(|n|-1)}{2} + |n|\|A\|^{-2}\left(e^{\|A\|} - \|A\| - 1 \right) \right] \|A\|_2^2
\end{aligned}$$

implies

$$\begin{aligned}
&\sum_{n=-\infty}^{\infty} |a_n| \left\| U^n - U_0^n - \frac{d}{ds}\Big|_{s=0} U_s^n \right\|_1 \\
&\leq \sum_{n=1}^{\infty} (|a_n| + |a_{-n}|) \left[\frac{n(n-1)}{2} + n\|A\|^{-2}\left(e^{\|A\|} - \|A\| - 1 \right) \right] \|A\|_2^2 < \infty.
\end{aligned}$$

Therefore the series in (2.26) converges in trace norm and hence $\left\{\Phi(U)-\Phi(U_0)-\frac{d}{ds}\Big|_{s=0}\Phi(U_s)\right\}$ is trace class and furthermore

$$\mathrm{Tr}\left\{\Phi(U)-\Phi(U_0)-\frac{d}{ds}\Big|_{s=0}\Phi(U_s)\right\}=\sum_{n=-\infty}^{\infty}a_n\ \mathrm{Tr}\left[U^n-U_0^n-\frac{d}{ds}\Big|_{s=0}U_s^n\right]. \tag{2.27}$$

Thus by combining Theorem 2.4.1 and (2.27) and applying Fubinni's theorem we get

$$\begin{aligned}\mathrm{Tr}\left\{\Phi(U)-\Phi(U_0)-\frac{d}{ds}\Big|_{s=0}\Phi(U_s)\right\}&=\sum_{n=-\infty}^{\infty}\int_0^{2\pi}(-n^2a_ne^{int})\eta(t)dt\\&=\int_0^{2\pi}\frac{d^2}{dt^2}\left\{\Phi(e^{it})\right\}\eta(t)dt.\end{aligned}$$

This completes the proof. □

Corollary 2.4.1. *If U and U_0 are two unitary operators in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $U-U_0\in\mathcal{B}_2(\mathcal{H})$. Then there exists an $L^1([0,2\pi])$- function η, unique up to an additive constant, such that for any $z\in\mathbb{C}$ with $|z|\neq 1$,*

$$\mathrm{Tr}\left\{(U-z)^{-1}-(U_0-z)^{-1}-\frac{d}{ds}\Big|_{s=0}(U_s-z)^{-1}\right\}=\int_0^{2\pi}\frac{d^2}{dt^2}\{(e^{it}-z)^{-1}\}\eta(t)dt.$$

CHAPTER 3

Second order trace formulae

3.1 Introduction

In Chapter 2, we have discussed the Koplienko-Neidhardt trace formula for pairs of unitaries (U, U_0), where the path considered by Neidhardt [42] is an unitary path, that is $U_s = e^{isA}U_0$ is an unitary operator for each $s \in \mathbb{R}$. In [26, Sect.10], Gesztesy, Pushnitski and Simon have discussed an alternative to Neidhardt's approach. In other words, they have considered the linear path $U_0 + t(U - U_0);\ 0 \leq t \leq 1$ instead of the unitary path $U_t = e^{itA}U_0;\ 0 \leq t \leq 1$ and proved that there exists a real distribution η on the unit circle $\mathbb{T}$ so that the formula

$$\operatorname{Tr}\left\{\phi(U) - \phi(U_0) - \frac{d}{ds}\left\{\phi\big(U_0 + s(U - U_0)\big)\right\}\bigg|_{s=0}\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\{p(e^{it})\}\ \eta(e^{it}, U_0, U)\ \frac{dt}{2\pi} \quad (3.1)$$

holds, for every complex polynomial $p(z) = \sum\limits_{k=0}^{n} a_k z^k;\ n \geq 0;\ a_k, z \in \mathbb{C}$. In this connection, Gesztesy et al. posed an open question in [26, Open Question 11.2] which says the following:

$$\textit{Is the above distribution } \eta \textit{ in } (3.1) \textit{ an } L^1(\mathbb{T}) - \textit{function?} \quad (3.2)$$

In 2012, Potapov and Sukochev provided an affirmative answer to the question mentioned above in [56]. In fact, they prove the following interesting theorem in [56].

Theorem 3.1.1. *(see [56, Theorem 1]) Let U and U_0 be two contractions in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $V := U - U_0 \in \mathcal{B}_2(\mathcal{H})$. Denote $U_s = U_0 + sV,\ s \in [0,1]$. Then for any complex polynomial $p(\cdot)$,*

$$\left\{ p(U) - p(U_0) - \frac{d}{ds}\bigg|_{s=0} \{p(U_s)\} \right\} \in \mathcal{B}_1(\mathcal{H})$$

and there exists an $L^1(\mathbb{T})$-function η (unique up to an analytic term) such that

$$\operatorname{Tr}\left\{ p(U) - p(U_0) - \frac{d}{ds}\bigg|_{s=0} \{p(U_s)\} \right\} = \int_{\mathbb{T}} p''(z)\eta(z)dz. \tag{3.3}$$

Moreover, for every given $\epsilon > 0$, we can choose the function η satisfying (3.3) in such a way so that

$$\|\eta\|_{L^1(\mathbb{T})} \leq (1+\epsilon)\ \|V\|_2^2. \tag{3.4}$$

It is worth mentioning that Dykema and Skripka [24] used the concept of unitary dilation to achieve some perturbation formulas for traces on normed ideals in semi-finite von Neumann algebra setting.

The following are the main contributions in this chapter.

- First of all, we supply a new proof of the above Theorem 3.1.1 whenever U_0 is a normal contraction and U is a contraction such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$ (see Theorem 3.5.1 and 3.5.3), we believe for the first time, using the idea of finite-dimensional approximation method as in the works of Voiculescu, Sinha and Mohapatra, referred to earlier which in particular provides an affirmative answer to the above question (3.2).

- Consequently, using the Schäffer matrix unitary dilation we also prove Theorem 3.1.1 corresponding to a class of pairs of contractions (T, T_0) such that $T - T_0 \in \mathcal{B}_2(\mathcal{H})$ (see Theorem 3.6.2 and Theorem 3.6.3).

- Next, by using our main theorem and using the Cayley transform of self-adjoint operators, we obtain the Koplienko trace formula corresponding to a pair of self-adjoint operators (H, H_0) with the same domain in $\mathcal{H}$ and under the assumption that $(H-z)^{-1} - (H_0 - z)^{-1} \in \mathcal{B}_2(\mathcal{H})$ for some z with $\operatorname{Im} z \neq 0$ (see Theorem 3.7.1).

- Moreover, by using Theorem 3.1.1 we prove the Koplienko trace formula for a pair of maximal dissipative operators (L, L_0) under the assumption $(L+i)^{-1}-(L_0+i)^{-1} \in \mathcal{B}_2(\mathcal{H})$ (see Theorem 3.8.1) for the first time.

- At the end, using the idea of finite-dimensional approximation method, we have extended the Koplienko-Neidhardt trace formula for a class of pairs of contractions (T, T_0) via multiplicative path (see Theorem 3.9.1).

The significant differences between our method and the method applied in [26, 56] are the following.

- Our approach in this chapter is different from that of [26, 56] and is probably closer to Koplienko and Neidhardt's original approach (see [31, 42]). In [56], the authors proved Krein type formula (see [56, Theorem 6]) to obtain Theorem 3.1.1 by approximating the perturbation operator (and not the initial operator) via trace class operators but still, they were in an infinite-dimensional setting to deal with the problem which makes a major contrast in comparison to our context. In other words, in our setting, we reduce the problem into a finite-dimensional one by truncating both the initial operator and the perturbation operator simultaneously via finite-dimensional projections $\{P_n\}$ (see Theorem 3.4.5 and 3.4.6).

- Moreover, in our setting, we calculate the shift function explicitly by performing integration by-parts and using semi-spectral measures for contractions (see Theorem 3.3.3 and 3.3.4), and it is one of the significant steps in our context to get the shift function in an infinite-dimensional case which is not the principle essence in the approach mentioned in [26, 56].

- Furthermore, using our approach we obtain a slightly better upper bound of the $L^1(\mathbb{T})$-norm of η (see Theorem 3.5.1 and Theorem 3.5.3) compared to (3.4) in Theorem 3.1.1.

The rest of the chapter is organized as follows: Section 3.2 deals with some well-known concepts/results that are essential in the later sections. In Section 3.3, we give the proof of the Koplienko trace formula and the Koplienko-Neidhardt trace formula for pairs of contractions when $dim\ \mathcal{H} < \infty$. Section 3.4 is devoted to reducing the problem into finite dimensions, and in Section 3.5, we prove the required trace formula by appropriate limiting argument. Consequently, in Section 3.6, we prove the trace formula for a class of pairs of contractions. Section 3.7 and Section 3.8 deal with the trace formula for a pair of self-adjoint operators and maximal dissipative operators respectively. At the end, in Section 3.9, we prove the Koplienko-Neidhardt trace for formula for a class of pairs of contractions via multiplicative path.

3.2 Preliminaries

For $1 \leq p \leq \infty$, the Hardy space $H^p(\mathbb{T})$ stand for the set $\{f \in L^p(\mathbb{T}) : \hat{f}(n) = 0, \text{ for all } n < 0\}$. One of the basic facts about $H^p(\mathbb{T})$ spaces is that they have preduals (see [25, Theorem 4.15]). In particular, $H^\infty(\mathbb{T})$ is isometrically isomorphic to the dual of the factor-space $L^1(\mathbb{T})/H^1(\mathbb{T})$ and furthermore, for every $f \in L^1(\mathbb{T})$, we have

$$\|[f]\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} = \sup_{\|g\|_{H^\infty(\mathbb{T})} \leq 1} \left| \int_{\mathbb{T}} g(z)f(z)dz \right|.$$

Now we denote the set of all complex polynomials by $\mathcal{P}(\mathbb{T})$. It is important to note that the supremum in the above equality can be taken over the set $\mathcal{P}(\mathbb{T})$. In other words, we have the following result

Lemma 3.2.1. *For every $f \in L^1(\mathbb{T})$, the equality*

$$\|[f]\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} = \sup_{g \in \mathcal{P}(\mathbb{T});\ \|g\|_{H^\infty} \leq 1} \left| \int_{\mathbb{T}} g(z)f(z)dz \right|$$

holds, where $\mathcal{P}(\mathbb{T})$ is the set of all complex polynomials.

The proof of Lemma 3.2.1 is available in [56, Lemma 5], and we need it in our context to calculate the norm on the factor space $L^1(\mathbb{T})/H^1(\mathbb{T})$ in later sections. Moreover, to prove our main results, we need the following fundamental estimate, which is obtained in [30, Theorem 6.1] (see also [50, Theorem 4.2 and (3.2)]).

Theorem 3.2.2. *If $f \in \mathcal{P}(\mathbb{T})$ then, for all contractions T, T_0 on $\mathcal{H}$,*

$$\begin{aligned} \|f(T) - f(T_0)\|_2 &\leq \|f'\|_\infty \, \|T - T_0\|_2 \qquad \text{if } T - T_0 \in \mathcal{B}_2(\mathcal{H}), \\ \text{and } \|f(T)X - Xf(T_0)\|_2 &\leq \|f'\|_\infty \, \|TX - XT_0\|_2 \qquad \text{if } X \in \mathcal{B}_2(\mathcal{H}), \end{aligned} \tag{3.5}$$

where $\|f'\|_\infty = \sup_{t \in [0, 2\pi)} |f'(e^{it})|$.

3.3 Trace formula in finite dimension

We begin the section with the following differentiation formula for monomials of contractions that can be established directly by definition of the Gâteaux derivative (with convergence in the operator norm).

Lemma 3.3.1. *Let T and T_0 be two contractions in an infinite dimensional separable Hilbert space $\mathcal{H}$. Let $V = T - T_0$, $T_s = T_0 + sV$, $s \in [0,1]$, and $p(z) = z^r$ $(r \geq 2), z \in \mathbb{T}$. Then*

$$\frac{d}{ds}\{p(T_s)\} = \sum_{j=0}^{r-1} T_s^{r-j-1} V T_s^j. \tag{3.6}$$

Proof. For $p(z) = z^r$ $(r \geq 2)$, $z \in \mathbb{T}$, we have

$$\frac{p(T_{s+h}) - p(T_s)}{h} = \frac{1}{h}\sum_{j=0}^{r-1} T_{s+h}^{r-j-1}(T_{s+h} - T_s)T_s^j = \sum_{j=0}^{r-1} T_{s+h}^{r-j-1} V T_s^j, \tag{3.7}$$

and hence

$$\left\| \frac{p(T_{s+h}) - p(T_s)}{h} - \sum_{j=0}^{r-1} T_s^{r-j-1} V T_s^j \right\| \leq |h| \left\{ \sum_{j=0}^{r-2} \sum_{k=0}^{r-j-2} \|T_s + hV\|^{r-j-k-2} \|V\| \|T_s\|^k \|V\| \|T_s\|^j \right\},$$

which converges to 0 as $h \longrightarrow 0$. This completes the proof. □

The following lemma essentially obtained in Theorem 2.2.2 whenever $A \in \mathcal{B}_2(\mathcal{H})$ is self-adjoint and T_0 is a unitary operator by using the definition of the Gâteaux derivative. But if we consider $A, T_0 \in \mathcal{B}(\mathcal{H})$, then the similar proof is also valid for the pair (A, T_0). Indeed, here we also give the proof for the reader's convenience.

Lemma 3.3.2. *Let (A, T_0) be a pair of bounded linear operator in an infinite dimensional separable Hilbert space $\mathcal{H}$. Let $T_s = e^{isA}T_0$, $s \in \mathbb{R}$, and $p(z) = z^r$ $(r \in \mathbb{Z}), z \in \mathbb{T}$. Then*

$$\frac{d}{ds}\{p(T_s)\} = \begin{cases} \sum\limits_{j=0}^{r-1} T_s^{r-j-1}(iA)T_s^{j+1} & \text{if } r \geq 1 \\ 0 & \text{if } r = 0 \\ -\sum\limits_{j=0}^{|r|-1} (T_s^*)^{|r|-j}(iA^*)(T_s^*)^j & \text{if } r \leq -1 \end{cases} \tag{3.8}$$

Proof. For $p(\lambda) = \lambda^r$ $(r \geq 1)$, $\lambda \in \mathbb{T}$, we have

$$\frac{p(T_{s+h}) - p(T_s)}{h} = \frac{1}{h}\sum_{k=0}^{r-1} T_{s+h}^{r-k-1}\left[T_{s+h} - T_s\right] T_s^k = \frac{1}{h}\sum_{k=0}^{r-1} T_{s+h}^{r-k-1}\left[e^{ihA} - I\right] T_s^{k+1},$$

which converges in operator norm to

$$\sum_{k=0}^{r-1} T_s^{r-k-1}\,(iA)\,T_s^{k+1} \quad \text{as} \quad h \to 0.$$

Similarly for $p(\lambda) = \lambda^r$ $(r \leq -1)$, $\lambda \in \mathbb{T}$, we have

$$\begin{aligned}\frac{p(T_{s+h}) - p(T_s)}{h} &= \frac{1}{h}\sum_{k=0}^{|r|-1} (T_{s+h}^*)^{|r|-k-1}\left[T_{s+h}^* - T_s^*\right](T_s^*)^k \\ &= \frac{1}{h}\sum_{k=0}^{|r|-1} (T_{s+h}^*)^{|r|-k-1}(T_s^*)\left[e^{-ihA} - I\right](T_s^*)^k,\end{aligned}$$

which again converges in operator norm to

$$-\sum_{k=0}^{r-1} (T_s^*)^{|r|-k}(iA)(T_s^*)^k \quad \text{as} \quad h \to 0.$$

□

The following theorem states Koplienko trace formula for pairs of contractions via linear path in finite dimension.

Theorem 3.3.3. *Let (N, N_0) be a pair of contractions on a finite dimensional Hilbert space $\mathcal{H}$, and $V = N - N_0$. Let $N_s = N_0 + sV$, $s \in [0,1]$ and $p(\cdot)$ be any complex polynomial. Then there exists a $L^1(\mathbb{T})$-function η such that*

$$\text{Tr}\left\{p(N) - p(N_0) - \frac{d}{ds}\Big|_{s=0}\{p(N_s)\}\right\} = \int_{\mathbb{T}} p''(z)\eta(z)dz, \tag{3.9}$$

where $p(\cdot)$ is any complex polynomial and

$$\eta(z) = \int_0^1 \text{Tr}\left[V\left\{\mathcal{E}_0(Arg(z)) - \mathcal{E}_s(Arg(z))\right\}\right]ds, \; z \in \mathbb{T}, \tag{3.10}$$

where $\mathcal{E}_s(\cdot)$ and $\mathcal{E}_0(\cdot)$ are the semi-spectral measures corresponding to the contractions N_s and N_0 respectively and $Arg(z)$ is the principle argument of z. Furthermore, the class of all η's satisfying (3.9) corresponds to a unique element $[\eta] \in L^1(\mathbb{T})/H^1(\mathbb{T})$ such that

$$\|[\eta]\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} \leq \frac{1}{2}\,\|V\|_2^2. \tag{3.11}$$

Proof. It will be sufficient to prove the theorem for $p(z) = z^r$, $z \in \mathbb{T}$. Note that for $r = 0$ or 1, both sides of (3.12) are identically zero. By using the cyclicity of trace, applying Lemma 3.3.1, and noting that the trace now is a finite sum, we have that for $p(z) = z^r$ $(r \geq 2), z \in \mathbb{T}$,

$$\operatorname{Tr}\left\{p(N) - p(N_0) - \frac{d}{ds}\Big|_{s=0}\{p(N_s)\}\right\} = \operatorname{Tr}\left\{\int_0^1 \frac{d}{ds}\{p(N_s)\}\, ds\right\} - \operatorname{Tr}\left\{\frac{d}{ds}\Big|_{s=0}\{p(N_s)\}\right\}$$
$$= \int_0^1 \operatorname{Tr}\left\{\sum_{j=0}^{r-1} N_s^{r-j-1} V N_s^j\right\} ds - \int_0^1 \operatorname{Tr}\left\{\sum_{j=0}^{r-1} N_0^{r-j-1} V N_0^j\right\} ds$$
$$= r\int_0^1 \left[\operatorname{Tr}\left\{V\left(N_s^{r-1} - N_0^{r-1}\right)\right\}\right] ds = \operatorname{Tr}\left\{rV\int_0^1 ds \int_0^{2\pi} e^{i(r-1)t}\left[\mathcal{E}_s(dt) - \mathcal{E}_0(dt)\right]\right\},$$

where $\mathcal{E}_s(\cdot)$ and $\mathcal{E}_0(\cdot)$ are the semi-spectral measures corresponding to the contractions N_s and N_0 respectively (see (1.13) and (1.14) in Section 1.6). Next by performing integration by-parts we have that

$$\operatorname{Tr}\left\{p(N) - p(N_0) - \frac{d}{ds}\Big|_{s=0}\{p(N_s)\}\right\}$$
$$= \operatorname{Tr}\left\{rV\int_0^1 ds\left(e^{i(r-1)t}\left[\mathcal{E}_s(t) - \mathcal{E}_0(t)\right]\Big|_{t=0}^{2\pi} - i(r-1)\int_0^{2\pi} e^{i(r-1)t}\left[\mathcal{E}_s(t) - \mathcal{E}_0(t)\right]dt\right)\right\}$$
$$= ir(r-1)\int_0^{2\pi} e^{i(r-1)t}\left\{\int_0^1 \operatorname{Tr}[V\{\mathcal{E}_0(t) - \mathcal{E}_s(t)\}]ds\right\}dt,$$

which by substituting $z = e^{it}$, $t \in [0, 2\pi]$ and $dt = \dfrac{dz}{iz}$ yields

$$\operatorname{Tr}\left\{p(N) - p(N_0) - \frac{d}{ds}\Big|_{s=0}\{p(N_s)\}\right\}$$
$$= \int_{\mathbb{T}} r(r-1)z^{r-2}\left\{\int_0^1 \operatorname{Tr}[V\{\mathcal{E}_0(Arg(z)) - \mathcal{E}_s(Arg(z))\}]\, ds\right\} dz = \int_{\mathbb{T}} p''(z)\eta(z)dz,$$

where $Arg(z)$ is the principle argument of z and we have set

$$\eta(z) = \int_0^1 \operatorname{Tr}\left[V\left\{\mathcal{E}_0(Arg(z)) - \mathcal{E}_s(Arg(z))\right\}\right]ds, \; z \in \mathbb{T}.$$

Let f be a complex polynomial on $\mathbb{T}$, and set $g(e^{it}) = \int_0^t f(e^{is})ie^{is}ds$, $t \in [0, 2\pi]$. Next we observe that $g(e^{i2\pi}) = g(e^{i0}) = 0$, and $\frac{d}{dt}\{g(e^{it})\} = ie^{it}f(e^{it})$. Now by using the above expression (3.10) of η and using Fubini's theorem to interchange the orders of integration and integrating by-parts, we have that

$$\int_{\mathbb{T}} f(z)\eta(z)dz = \int_0^{2\pi} f(e^{it})\eta(e^{it})ie^{it}dt = \int_0^{2\pi} \frac{d}{dt}\{g(e^{it})\}\eta(e^{it})dt$$
$$= \int_0^{2\pi} \frac{d}{dt}\{g(e^{it})\}\left(\int_0^1 \operatorname{Tr}\left[V\left\{\mathcal{E}_0(t) - \mathcal{E}_s(t)\right\}\right] ds\right) dt$$

$$= \int_0^1 ds \int_0^{2\pi} \frac{d}{dt}\{g(e^{it})\} \ \mathrm{Tr}\left[V\left\{\mathcal{E}_0(t) - E_s(t)\right\}\right] dt$$
$$= \int_0^1 ds \left(g(e^{it}) \ \mathrm{Tr}\left[V\left\{\mathcal{E}_0(t) - \mathcal{E}_s(t)\right\}\right]\Big|_{t=0}^{2\pi} - \int_0^{2\pi} g(e^{it}) \ \mathrm{Tr}\left[V\left\{\mathcal{E}_0(dt) - \mathcal{E}_s(dt)\right\}\right]\right)$$
$$= -\int_0^1 ds \int_0^{2\pi} g(e^{it}) \ \mathrm{Tr}\left[V\left\{\mathcal{E}_0(dt) - \mathcal{E}_s(dt)\right\}\right] = \int_0^1 ds \ \mathrm{Tr}\left[V\left\{g(N_s) - g(N_0)\right\}\right].$$

Therefore using Theorem 3.2.2 we get

$$\left|\int_{\mathbb{T}} f(z)\eta(z)dz\right| = \left|\int_0^1 ds \ \mathrm{Tr}\left[V\left\{g(N_s) - g(N_0)\right\}\right]\right| \le \int_0^1 ds \left|\mathrm{Tr}\left[V\left\{g(N_s) - g(N_0)\right\}\right]\right|$$
$$\le \int_0^1 \|V\|_2 \|g(N_s) - g(N_0)\|_2 \le \int_0^1 \|g'\|_\infty \|V\|_2 \|N_s - N_0\|_2 \le \|f\|_\infty \|V\|_2^2 \int_0^1 s \ ds \ = \frac{1}{2}\|f\|_\infty \|V\|_2^2,$$

and hence by using Lemma 3.2.1 we conclude that

$$\|[\eta]\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} = \sup_{f\in\mathcal{P}(\mathbb{T});\ \|f\|_{H^\infty(\mathbb{T})}\le 1} \left|\int_{\mathbb{T}} f(z)\eta(z)dz\right| \le \frac{1}{2} \ \|V\|_2^2.$$

This completes the proof.

□

The following theorem states the Koplienko-Neidhardt trace formula for pairs of contractions via multiplicative path in finite dimension.

Theorem 3.3.4. *Let T_0 be a contraction in a finite dimensional Hilbert space $\mathcal{H}$ and let $A = A^*$ $\in \mathcal{B}(\mathcal{H})$. Denote $T_s = e^{isA}T_0,\ s \in [0,1]$, and $T = T_1$. Then there exists a $L^1([0,2\pi])$-function $\tilde{\eta}$ such that*

$$\mathrm{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0}\{p(T_s)\}\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\left\{p(e^{it})\right\}\tilde{\eta}(t)dt, \tag{3.12}$$

where $p(\cdot)$ is any complex polynomial on $\mathbb{T}$ with complex coefficients and

$$\tilde{\eta}(t) = \int_0^1 \mathrm{Tr}\left[A\left\{\mathcal{F}_0(t) - \mathcal{F}_s(t)\right\}\right] ds,\ t \in [0,2\pi], \tag{3.13}$$

where $\mathcal{F}_s(\cdot)$ and $\mathcal{F}_0(\cdot)$ are the semi-spectral measures corresponding to the contractions T_s and T_0 respectively. Moreover,

$$\|[\tilde{\eta}]\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} \le \frac{1}{2} \ \|A\|_2^2. \tag{3.14}$$

Proof. It will be sufficient to prove the theorem for $p(z) = z^r$ $, r \in \mathbb{N} \cup \{0\}, z \in \mathbb{T}$. Note that for $r = 0$, both sides of (3.12) are identically zero. Let $\mathcal{F}_s(\cdot)$ and $\mathcal{F}_0(\cdot)$ are the semi-spectral measures corresponding to the contractions T_s and T_0 respectively (see (1.13) and (1.14) in Section 3.2). By using the cyclicity of trace, applying Lemma 3.3.2, and noting that the trace now is a finite sum, we have that for $p(z) = z^r$ $(r \geq 1), z \in \mathbb{T}$,

$$\begin{aligned}
&\operatorname{Tr}\left\{p(T_1) - p(T_0) - \frac{d}{ds}p(T_s)\Big|_{s=0}\right\} = \operatorname{Tr}\left\{\int_0^1 \left(\frac{d}{ds}p(T_s) - \frac{d}{dt}p(T_t)\Big|_{t=0}\right) ds\right\} \\
&= \operatorname{Tr}\left\{\int_0^1 \left(\sum_{j=0}^{r-1} T_s^{r-j-1}(iA)T_s^{j+1} - \sum_{j=0}^{r-1} T_0^{r-j-1}(iA)T_0^{j+1}\right) ds\right\} \\
&= \operatorname{Tr}\left\{(ir)A \int_0^1 (T_s^r - T_0^r)\, ds\right\} \\
&= \operatorname{Tr}\left\{(ir)A \int_0^1 ds \int_0^{2\pi} e^{irt}\Big(\mathcal{F}_s(dt) - \mathcal{F}_0(dt)\Big)\right\} \\
&= \operatorname{Tr}\left[(ir)A \int_0^1 ds \left\{e^{irt}\big(\mathcal{F}_s(t) - \mathcal{F}_0(t)\big)\Big|_{t=0}^{2\pi} - ir\int_0^{2\pi} e^{irt}\big(\mathcal{F}_s(t) - \mathcal{F}_0(t)\big)dt\right\}\right] \\
&= \int_0^{2\pi} (ir)^2 e^{irt}\left[\int_0^1 \operatorname{Tr}\Big\{A\big(\mathcal{F}_0(t) - \mathcal{F}_s(t)\big)\Big\}ds\right] dt = \int_0^{2\pi} \frac{d^2}{dt^2}\Big\{p(e^{it})\Big\}\eta(t)dt.
\end{aligned}$$

Therefore we have the formula (3.12) by setting

$$\tilde{\eta}(t) = \int_0^1 \operatorname{Tr}\big\{A[\mathcal{F}_0(t) - \mathcal{F}_s(t)]\big\}ds.$$

By repeating the similar argument as done in Theorem 3.3.3 we obtain (3.14). This completes the proof. □

Remark 3.3.5. *It is easy to observe that the function $\tilde{\eta}$ in (3.13) is real-valued. Also it is worth mentioning that, if we consider the polynomial $p(z) = z^r$ for $r \leq -1$, then by performing similar calculations as done in the proof of Theorem 2.2.2, we also obtain the formula (3.12) along with the same spectral shift function $\tilde{\eta}$ as in (3.14). Therefore the identity (3.12) holds for every trigonometric polynomial and hence by the uniqueness of the Fourier series we conclude that the spectral shift function $\tilde{\eta}(\cdot)$ is unique up to an additive constant. Moreover, the formula (3.12) can also be extended for the class $\mathcal{F}_2(\mathbb{T})$.*

3.4 Reduction to finite dimension

We begin the section by stating (without proof) the approximation theorem which is essential in our context to reduce the problem into a finite dimensional one. Note that the following theorem is a special case of Theorem 2.2 in [21]. Moreover, it is also worth mentioning that Voiculescu [74] had earlier obtained related (though not the same) results.

Theorem 3.4.1. *(See [21, Theorem 2.2]) Let (A_1, A_2) be a pair of commuting bounded self-adjoint operators in an infinite-dimensional separable Hilbert space $\mathcal{H}$. Then there exists a sequence $\{P_k\}$ of finite-rank projections such that, for $i = 1, 2$*

$$P_k \uparrow I, \quad \text{and} \quad \|[A_i, P_k]\|_2 \longrightarrow 0, \text{ as } k \longrightarrow \infty. \tag{3.15}$$

Using the above theorem we have the following useful lemmas which will be useful to reduce the problem into a finite dimensional case.

Lemma 3.4.2. *Let (H_1, H_2) be a pair of commuting bounded self-adjoint operators in an infinite-dimensional separable Hilbert space $\mathcal{H}$. Let $A \in \mathcal{B}_2(\mathcal{H})$ be a self-adjoint operator and let $B \in \mathcal{B}_2(\mathcal{H})$. Then for $i = 1, 2$, there exists a sequence $\{P_k\}$ of finite rank projections such that $P_k \uparrow I$, and*

$$\left\|P_k^\perp H_i P_k\right\|_2, \quad \left\|P_k^\perp A P_k\right\|_2, \quad \left\|P_k^\perp B P_k\right\|_2, \left\|P_k^\perp B^* P_k\right\|_2 \longrightarrow 0 \text{ as } k \longrightarrow \infty.$$

Proof. Now by applying Theorem 3.4.1 corresponding to the pair (H_1, H_2), there exists a sequence $\{P_k\}$ finite rank projections such that $P_k \uparrow I$, and

$$\left\|P_k^\perp H_i P_k\right\|_2 \longrightarrow 0 \text{ as } k \longrightarrow \infty \quad \text{for} \quad i = 1, 2.$$

Let $\sum_{j=1}^{\infty} \lambda_j \langle \cdot, e_j \rangle f_j$ and $\sum_{j=1}^{\infty} \mu_j \langle \cdot, g_j \rangle h_j$ be the corresponding canonical decomposition of A and B respectively, where $\sum_{j=1}^{\infty} \lambda_j^2 < \infty$, $\sum_{j=1}^{\infty} \mu_j^2 < \infty$ and $\{e_j\}$, $\{f_j\}$, $\{g_j\}$ and $\{h_j\}$ are set of orthonormal vectors. Now given $n \in \mathbb{N}$, there exists $L_n \in \mathbb{N}$ such that

$$\sum_{j=L_n+1}^{\infty} \lambda_j^2 < \frac{1}{n}, \text{ and } \sum_{j=L_n+1}^{\infty} \mu_j^2 < \frac{1}{n}.$$

Set $A_{L_n} = \sum_{j=1}^{L_n} \lambda_j \langle \cdot, e_j \rangle f_j$, $A_{L_n}^* = \sum_{j=1}^{L_n} \lambda_j \langle \cdot, f_j \rangle e_j$, $B_{L_n} = \sum_{j=1}^{L_n} \mu_j \langle \cdot, g_j \rangle h_j$, $B_{L_n}^* = \sum_{j=1}^{L_n} \mu_j \langle \cdot, h_j \rangle g_j$, and $\epsilon_n = \min\left\{ \frac{1}{n}, \frac{\frac{1}{n}}{\sum_{j=1}^{L_n} \lambda_j}, \frac{\frac{1}{n}}{\sum_{j=1}^{L_n} \mu_j} \right\}$. Since $P_k \uparrow I$ as $k \to \infty$, then there exists a natural number a_n

such that for each $f \in \{e_1, e_2, \dots, e_{L_n}\} \cup \{f_1, f_2, \dots, f_{L_n}\} \cup \{g_1, g_2, \dots, g_{L_n}\} \cup \{h_1, h_2, \dots, h_{L_n}\}$ we have

$$\|(I - P_k)f\| < \epsilon_n \quad \forall\, k \geq a_n.$$

Next we choose $a_n \in \mathbb{N}$ such that $a_n < a_{n+1}$ for each $n \in \mathbb{N}$. Therefore corresponding to the sub-sequence $\{P_{a_n}\}$, we have for $i = 1, 2,$

$$\begin{aligned} &\left\|P_{a_n}^{\perp} H_i P_{a_n}\right\|_2 \longrightarrow 0, \\ &\left\|P_{a_n}^{\perp} A P_{a_n}\right\|_2 \leq \left\|P_{a_n}^{\perp}(A - A_{L_n})P_{a_n}\right\|_2 + \left\|P_{a_n}^{\perp} A_{L_n} P_{a_n}\right\|_2 \\ &\qquad \leq \|A - A_{L_n}\|_2 + \left\|P_{L_n}^{\perp} A_{L_n}\right\|_2 < \frac{1}{n} + \epsilon_n \left(\sum_{j=1}^{L_n} \lambda_j^2\right)^{\frac{1}{2}} \leq \frac{2}{n} \longrightarrow 0 \quad \text{as} \quad n \longrightarrow \infty. \end{aligned}$$

Similarly we have

$$\left\|P_{a_n}^{\perp} A^* P_{a_n}\right\|_2 < \frac{1}{n} + \epsilon_n \left(\sum_{j=1}^{L_n} \lambda_j^2\right)^{\frac{1}{2}} \leq \frac{2}{n} \longrightarrow 0, \quad \left\|P_{a_n}^{\perp} B P_{a_n}\right\|_2 < \frac{1}{n} + \epsilon_n \left(\sum_{j=1}^{L_n} \mu_j^2\right)^{\frac{1}{2}} \leq \frac{2}{n} \longrightarrow 0,$$

$$\text{and} \quad \left\|P_{a_n}^{\perp} B^* P_{a_n}\right\|_2 < \frac{1}{n} + \epsilon_n \left(\sum_{j=1}^{L_n} \mu_j^2\right)^{\frac{1}{2}} \leq \frac{2}{n} \longrightarrow 0 \quad \text{as} \quad n \longrightarrow \infty.$$

This complete the proof. □

Lemma 3.4.3. *Let N_0 be a normal contraction on a separable Hilbert space $\mathcal{H}$, and let $V \in \mathcal{B}_2(\mathcal{H})$. Let $T_0 = N_0 + V$ and $A = A^* \in \mathcal{B}_2(\mathcal{H})$. Set $T_s = e^{isA}T_0$, $s \in [0,1]$ and $T = T_1$. Then there exists a sequence $\{P_n\}$ of finite rank projections such that for every $k \in \mathbb{N}$, each of the following terms*

$$\begin{aligned} &(i)\ \ \|P_n^{\perp} N_0 P_n\|_2, \quad (ii)\ \ \|P_n^{\perp} V\|_2, \quad (iii)\ \ \|P_n^{\perp} V^*\|_2, \quad (iv)\ \ \left\|\left(T^k - T_n^k\right) P_n\right\|_2, \\ &(v)\ \ \left\|\left(T_0^k - T_{0,n}^k\right) P_n\right\|_2, \quad (vi)\ \ \left\|P_n^{\perp}\left(e^{iA} - I\right)\right\|_2, (vii)\ \ \left\|P_n\left(e^{iA} - e^{iA_n}\right)\right\|_2, \\ &(viii)\ \ \left\|\left(e^{iA} - iA - e^{iA_n} + iA_n\right) P_n\right\|_1, \quad \text{and} \quad (ix)\ \ \left\|\left(e^{iA} - iA - I\right) P_n^{\perp}\right\|_1 \end{aligned}$$

converges to zero as $n \longrightarrow \infty$, where $A_n = P_n A P_n$, $T_{0,n} = P_n T_0 P_n$, $T_n = e^{iA_n} T_{0,n}$ and $T_{s,n} = e^{isA_n} T_{0,n}$.

Proof. Since N_0 is a normal contraction, then $N_0 + N_0^*$ and $N_0 - N_0^*$ are two commuting self-adjoint operators on $\mathcal{H}$. Therefore by applying Lemma 3.4.2 corresponding to the pair $(N_0 + N_0^*, N_0 - N_0^*)$, there exists a sequence $\{P_n\}$ of finite rank projections such that

$$\left\|P_n^{\perp}(N_0 + N_0^*)P_n\right\|_2, \left\|P_n^{\perp}(N_0 - N_0^*)P_n\right\|_2, \left\|P_n^{\perp} A\right\|_2, \left\|P_n^{\perp} V\right\|_2, \left\|P_n^{\perp} V^*\right\|_2 \longrightarrow 0 \text{ as } n \longrightarrow \infty,$$

which immediately implies that

$$\left\|P_n^{\perp}N_0P_n\right\|_2, \left\|P_n^{\perp}N_0^*P_n\right\|_2, \left\|P_n^{\perp}T_0P_n\right\|_2, \left\|P_n^{\perp}T_0^*P_n\right\|_2 \longrightarrow 0 \text{ as } n \longrightarrow \infty. \tag{3.16}$$

This conclude (*i*), (*ii*) and (*iii*). The proof of (*iv*), (*v*), (*vi*), (*vii*) and (*ix*) can be obtained similarly by mimicking the proof of Lemma 2.3.3. For (*viii*), consider the following

$$\begin{aligned}
&\left\|\left(e^{iA} - iA - e^{iA_n} + iA_n\right) P_n\right\|_1 \\
&= \left\| \sum_{k=2}^{\infty} \frac{1}{k!} \sum_{j=0}^{k-1} \left\{ (iA)^{k-j-1}(iA - iA_n)(iA_n)^j \right\} P_n \right\|_1 \\
&= \left\| \sum_{k=2}^{\infty} \frac{1}{k!} \left[\sum_{j=0}^{k-1} \left\{ (iA)^{k-j-1}(iA - iA_n)(iA_n)^j \right\} P_n \right] \right\|_1 \\
&= \left\| \sum_{k=2}^{\infty} \frac{1}{k!} \left[(iA)^{k-1} i\left(P_n^{\perp}AP_n\right) + i\left(P_n^{\perp}AP_n\right)(iA_n)^{k-1} + \sum_{j=1}^{k-2} \left\{ (iA)^{k-j-1} i\left(P_n^{\perp}AP_n\right)(iA_n)^j \right\} P_n \right] \right\|_1 \\
&= \sum_{k=2}^{\infty} \frac{1}{k!} \Big[\|A\|^{k-2}\|A\|_2 \left\|P_n^{\perp}AP_n\right\|_2 + \left\|P_n^{\perp}AP_n\right\|_2 \|A_n\|^{k-2}\|A_n\|_2 \\
&\qquad\qquad + \sum_{j=1}^{k-2} \left\{ \|A\|^{k-j-1} \left\|P_n^{\perp}AP_n\right\|_2 \|A_n\|^{j-1}\|A_n\|_2 \right\} \Big] \\
&= \left(\sum_{k=2}^{\infty} \frac{1}{(k-1)!} \|A\|^{k-2} \right) \|A\|_2 \left\|P_n^{\perp}AP_n\right\|_2 = \|A\|^{-1}\left(e^{\|A\|} - 1\right)\|A\|_2 \left\|P_n^{\perp}AP_n\right\|_2 \longrightarrow 0 \text{ as } n \longrightarrow \infty.
\end{aligned}$$

This completes the proof. □

Remark 3.4.4. *Note that the expressions (iv) and (v) in Lemma 3.4.3 also converge to zero as $n \longrightarrow \infty$ for any $k \in \mathbb{Z}$, where we interpret T^{-1} as the adjoint of T.*

The following two theorems show how the above Lemma 3.4.3 can be used to reduce the relevant problem into a finite-dimensional one.

Theorem 3.4.5. *Let N_0 be a normal contraction on a separable Hilbert space $\mathcal{H}$, and let $V \in \mathcal{B}_2(\mathcal{H})$. Let $N_s = N_0 + sV$, $s \in [0,1]$, $N = N_1$ and let $p(\cdot)$ be any complex polynomial. Then there exists a sequence $\{P_n\}$ of finite rank projections such that*

$$\left\| \left\{ p(N) - p(N_0) - \frac{d}{ds}\bigg|_{s=0} \{p(N_s)\} \right\} - \left\{ P_n \left(p(N_n) - p(N_{0,n}) - \frac{d}{ds}\bigg|_{s=0} \{p(N_{s,n})\} \right) P_n \right\} \right\|_1 \tag{3.17}$$

$\longrightarrow 0$ as $n \longrightarrow \infty$, where $N_n = P_nNP_n$, $N_{0,n} = P_nN_0P_n$, and $N_{s,n} = P_nN_sP_n$.

Proof. It will be sufficient to prove the theorem for $p(z) = z^r, r \in \mathbb{N}, z \in \mathbb{T}$. Note that for $r = 0$ or 1, the expressions inside the trace norm in (3.17) are identically zero. Let $r \geq 2$. Now by using the sequence $\{P_n\}$ of finite rank projections as obtained in Lemma 3.4.3, and using an expression similar to (3.6) in $\mathcal{B}(\mathcal{H})$, we have that

$$\begin{aligned}
&\left\| \Big(N^r - N_0^r - \sum_{j=0}^{r-1} N_0^{r-j-1} V N_0^j\Big) - P_n\Big(N_n^r - N_{0,n}^r - \sum_{j=0}^{r-1} N_{0,n}^{r-j-1} V N_{0,n}^j\Big) P_n \right\|_1 \\
&= \left\| \sum_{\substack{\alpha+\beta=r-1 \\ \alpha\geq 1 \ \& \ \beta\geq 0}} \Big[(N^\alpha - N_0^\alpha) V N_0^\beta - P_n\Big((N_n^\alpha - N_{0,n}^\alpha) V N_{0,n}^\beta\Big) P_n\Big] \right\|_1 \\
&= \Bigg\| \sum_{\substack{\alpha+\beta=r-1 \\ \alpha\geq 1 \ \& \ \beta\geq 0}} \Bigg[\Big\{(N^\alpha - N_n^\alpha) P_n V N_0^\beta + N^\alpha P_n^\perp V N_0^\beta + N_n^\alpha V P_n (N_0^\beta - N_{0,n}^\beta) + N_n^\alpha V P_n^\perp N_0^\beta\Big\} \\
&\quad - \Big\{(N_0^\alpha - N_{0,n}^\alpha) P_n V N_0^\beta + N_0^\alpha P_n^\perp V N_0^\beta + N_{0,n}^\alpha V P_n (N_0^\beta - N_{0,n}^\beta) + N_{0,n}^\alpha V P_n^\perp N_0^\beta\Big\}\Bigg]\Bigg\|_1 \\
&\leq \sum_{\substack{\alpha+\beta=r-1 \\ \alpha\geq 1 \ \& \ \beta\geq 0}} \Big\{\|(N^\alpha - N_n^\alpha) P_n\|_2 \|V\|_2 + \alpha \|V\|_2 \left(\|P_n^\perp V\|_2 + \|V P_n^\perp\|_2\right) + 2\|V\|_2 \|P_n (N_0^\beta - N_{0,n}^\beta)\|_2 \\
&\qquad + \|(N_0^\alpha - N_{0,n}^\alpha) P_n\|_2 \|V\|_2\Big\}.
\end{aligned} \tag{3.18}$$

Now using the estimates listed in Lemma 3.4.3 along with the Remark 3.4.4, we conclude that the expression in the right hand side of (3.18) converges to zero as $n \longrightarrow \infty$. This completes the proof. □

Theorem 3.4.6. *Let $T_0 = N_0 + V$ be a contraction on a separable Hilbert space $\mathcal{H}$, where N_0 is a bounded normal operator and $V \in \mathcal{B}_2(\mathcal{H})$. Let $A = A^* \in \mathcal{B}_2(\mathcal{H})$, $T_s = e^{isA} T_0$, $s \in [0,1]$, $T = T_1$ and $p(\cdot)$ be any trigonometric polynomial on $\mathbb{T}$ with complex coefficients. Then*

$$p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} p(T_s) \in \mathcal{B}_1(\mathcal{H}), \tag{3.19}$$

and there exists a sequence $\{P_n\}$ of finite rank projections in $\mathcal{H}$ such that

$$\left\| \left[\Big\{p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} p(T_s)\Big\} - P_n\Big\{p(T_n) - p(T_{0,n}) - \frac{d}{ds}\bigg|_{s=0} p(T_{s,n})\Big\} P_n\right] \right\|_1 \tag{3.20}$$

$\longrightarrow 0$ as $n \to \infty$, where $A_n = P_n A P_n$, $T_{0,n} = P_n T_0 P_n$, $T_n = e^{iA_n} T_{0,n}$ and $T_{s,n} = e^{isA_n} T_{0,n}$.

Proof. It will be sufficient to prove the theorem for $p(z) = z^r, r \in \mathbb{Z}, z \in \mathbb{T}$. The property (3.19) is trivial. Note that for $r = 0$, the expression inside the trace norm in (3.20) is identically zero.

For $r \geq 1$, using the sequence $\{P_n\}$ of finite rank projections as obtained in Lemma 3.4.3, and using an expression similar to (3.8) in $\mathcal{B}(\mathcal{H})$, we have that

$$\begin{aligned}
&\left[\left\{p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} p(T_s)\right\} - P_n\left\{p(T_n) - p(T_{0,n}) - \frac{d}{ds}\bigg|_{s=0} p(T_{s,n})\right\}P_n\right] \\
&= \left[\left\{T^r - T_0^r - \sum_{j=0}^{r-1} T_0^{r-j-1}(iA)T_0^{j+1}\right\} - P_n\left\{T_n^r - T_{0,n}^r - \sum_{j=0}^{r-1} T_{0,n}^{r-j-1}(iA_n)T_{0,n}^{j+1}\right\}P_n\right] \\
&= \sum_{\substack{\alpha+\beta=r \\ \alpha\geq 0\ \&\ \beta\geq 1}} \left[\left\{T^\alpha(e^{iA} - I)T_0^\beta - T_0^\alpha(iA)T_0^\beta\right\} - P_n\left\{T_n^\alpha P_n(e^{iA_n} - I)P_nT_{0,n}^\beta - T_{0,n}^\alpha(iA_n)T_{0,n}^\beta\right\}P_n\right] \\
&= \sum_{\substack{\alpha+\beta=r \\ \alpha\geq 0\ \&\ \beta\geq 1}} \Bigg[\left\{(T^\alpha - T_0^\alpha)(e^{iA} - I)T_0^\beta + T_0^\alpha(e^{iA} - iA - I)T_0^\beta\right\} \\
&\qquad - P_n\left\{\left(T_n^\alpha - T_{0,n}^\alpha\right)P_n(e^{iA_n} - I)P_nT_{0,n}^\beta + T_{0,n}^\alpha(e^{iA_n} - iA_n - I)T_{0,n}^\beta\right\}P_n\Bigg] \\
&= \sum_{\substack{\alpha+\beta=r \\ \alpha\geq 0\ \&\ \beta\geq 1}} \Bigg[\Bigg\{\left(T^\alpha - T_n^\alpha - T_0^\alpha + T_{0,n}^\alpha\right)P_n(e^{iA} - I)T_0^\beta + \left(T^\alpha - T_0^\alpha\right)P_n^\perp(e^{iA} - I)T_0^\beta \\
&\qquad + \left(T_n^\alpha - T_{0,n}^\alpha\right)P_n\left(e^{iA} - e^{iA_n}\right)T_0^\beta + \left(T_n^\alpha - T_{0,n}^\alpha\right)P_n\left(e^{iA_n} - I\right)P_n\left(T_0^\beta - T_{0,n}^\beta\right)\Bigg\} \\
&\quad - \Bigg\{(T_0^\alpha - T_{0,n}^\alpha)P_n\left(e^{iA} - iA - I\right)T_0^\beta + T_0^\alpha P_n^\perp\left(e^{iA} - iA - I\right)T_0^\beta \\
&\qquad + T_{0,n}^\alpha P_n\left(e^{iA} - iA - e^{iA_n} + iA_n\right)T_0^\beta + T_{0,n}^\alpha P_n(e^{iA_n} - iA_n - I)P_n\left(T_0^\beta - T_{0,n}^\beta\right)\Bigg\}\Bigg],
\end{aligned}$$

and hence we have the following estimate

$$\begin{aligned}
&\left\|\left[\left\{p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} p(T_s)\right\} - P_n\left\{p(T_n) - p(T_{0,n}) - \frac{d}{ds}\bigg|_{s=0} p(T_{s,n})\right\}P_n\right]\right\|_1 \\
&\leq \sum_{\substack{\alpha+\beta=r \\ \alpha\geq 0\ \&\ \beta\geq 1}} \Bigg[\left\|(T^\alpha - T_n^\alpha - T_0^\alpha - T_{0,n}^\alpha)P_n\right\|_2\left\|(e^{iA} - I)\right\|_2 + \left\|(T^\alpha - T_0^\alpha)\right\|_2\left\|P_n^\perp(e^{iA} - I)\right\|_2 \\
&+ \left\|\left(T_n^\alpha - T_{0,n}^\alpha\right)P_n\right\|_2\left\|P_n\left(e^{iA} - e^{iA_n}\right)\right\|_2 + 2\left\|P_n\left(e^{iA_n} - I\right)P_n\right\|_2\left\|P_n\left(T_0^\beta - T_{0,n}^\beta\right)\right\|_2 \\
&+ \left\|(T_0^\alpha - T_{0,n}^\alpha)P_n\right\|_2\left\|\left(e^{iA} - iA - I\right)\right\|_2 + \left\|P_n^\perp\left(e^{iA} - iA - I\right)\right\|_1 + \left\|P_n\left(e^{iA} - iA - e^{iA_n} + iA_n\right)\right\|_1 \\
&+ \left\|P_n(e^{iA_n} - iA_n - I)P_n\right\|_2\left\|P_n\left(T_0^\beta - T_{0,n}^\beta\right)\right\|_2\Bigg].
\end{aligned} \tag{3.21}$$

Finally, using the estimates listed in Lemma 3.4.3, we conclude that each term in the right hand side of (3.21) converges to zero as $n \longrightarrow \infty$. By repeating the similar calculations as above and using Lemma 3.4.3 and Remark 3.4.4 we conclude (3.20) for $p(z) = z^r, r \leq -1$.

□

Remark 3.4.7. *Note that, in the above Theorem 3.4.6 we prove the convergence of the expression in (3.20) in trace norm instead of taking the trace of the expression and show the convergence. In other words, the above Theorem 3.4.6 deals with the trace norm convergence which is stronger in comparison with the trace convergence as obtained in Theorem 2.3.6 and also we are dealing with pair of contractions (T, T_0) instead of pair unitaries (U, U_0).*

3.5 Existence of shift function in linear path

Now we are in a position to derive the trace formula corresponding to the pair of contractions (N, N_0), where N_0 is a normal operator. The following theorem is one of the main results in this section.

Theorem 3.5.1. *Let N and N_0 be two contraction operators in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that N_0 is normal and $V = N - N_0 \in \mathcal{B}_2(\mathcal{H})$. Denote $N_s = N_0 + sV$, $s \in [0,1]$. Then for any complex polynomial $p(\cdot)$, $\left\{p(N) - p(N_0) - \frac{d}{ds}\Big|_{s=0} \{p(N_s)\}\right\} \in \mathcal{B}_1(\mathcal{H})$ and there exists an $L^1(\mathbb{T})$-function η (unique up to an analytic term) such that*

$$\operatorname{Tr}\left\{p(N) - p(N_0) - \frac{d}{ds}\Big|_{s=0} \{p(N_s)\}\right\} = \int_{\mathbb{T}} p''(z)\eta(z)dz. \tag{3.22}$$

Moreover, for every given $\epsilon > 0$, we choose the function η satisfying (3.22) in such a way so that

$$\|\eta\|_{L^1(\mathbb{T})} \leq \left(\frac{1}{2} + \epsilon\right) \|V\|_2^2. \tag{3.23}$$

Proof. By Theorem 3.4.5 and Theorem 3.3.3, we have that

$$\begin{aligned}
&\operatorname{Tr}\left\{p(N) - p(N_0) - \frac{d}{ds}\Big|_{s=0} \{p(N_s)\}\right\} \\
&= \lim_{n\to\infty} \operatorname{Tr}\left\{P_n\left(p(N_n) - p(N_{0,n}) - \frac{d}{ds}\Big|_{s=0} \{p(N_{s,n})\}\right)P_n\right\} \\
&= \lim_{n\to\infty} \int_{\mathbb{T}} p''(z)\eta_n(z)dz,
\end{aligned} \tag{3.24}$$

where $N_n = P_nNP_n$, $N_{0,n} = P_nN_0P_n$, $N_{s,n} = P_nN_sP_n$, and $\eta_n(z)$ is given by (3.10), that is

$$\eta_n(z) = \int_0^1 \operatorname{Tr}\left[V_n\left\{\mathcal{E}_{0,n}\Big(Arg(z)\Big) - \mathcal{E}_{s,n}\Big(Arg(z)\Big)\right\}\right]ds, \ z \in \mathbb{T}, \tag{3.25}$$

where $\mathcal{E}_{s,n}(\cdot)$ and $\mathcal{E}_{0,n}(\cdot)$ are the semi-spectral measures corresponding to the contractions $N_{s,n}$ and $N_{0,n}$ respectively (see (1.13) and (1.14) in Section 3.2) and $V_n = P_n V P_n$. Moreover, from (3.11) it follows that

$$\left\|[\eta_n]\right\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} \leq \frac{1}{2}\, \|V_n\|_2^2. \tag{3.26}$$

Next we show that the sequence $\{\eta_n\}$ converges in some suitable sense. Indeed, by following the idea contained in [26, 31, 42] (see also [22, 18]), using the above expression (3.25) of η_n, using Fubini's theorem to interchange the orders of integration and integrating by-parts, we have for $f \in \mathcal{P}(\mathbb{T})$ and $g(e^{it}) = \int_0^t f(e^{is})\, ie^{is}ds,\ t \in [0, 2\pi]$ that

$$\begin{aligned}
&\int_{\mathbb{T}} f(z)\{\eta_n(z) - \eta_m(z)\}dz = \int_0^{2\pi} f(e^{it})\{\eta_n(e^{it}) - \eta_m(e^{it})\}\ ie^{it}dt\\
&= \int_0^{2\pi} \frac{d}{dt}\{g(e^{it})\}\left[\int_0^1 \operatorname{Tr}\left[V_n\left\{\mathcal{E}_{0,n}(t) - \mathcal{E}_{s,n}(t)\right\} - V_m\left\{\mathcal{E}_{0,m}(t) - \mathcal{E}_{s,m}(t)\right\}\right] ds\right] dt\\
&= \int_0^1 \left[\int_0^{2\pi} \frac{d}{dt}\{g(e^{it})\}\ \operatorname{Tr}\left[V_n\left\{\mathcal{E}_{0,n}(t) - \mathcal{E}_{s,n}(t)\right\} - V_m\left\{\mathcal{E}_{0,m}(t) - \mathcal{E}_{s,m}(t)\right\}\right] dt\right] ds\\
&= \int_0^1 \Bigg[g(e^{it})\ \operatorname{Tr}\left[V_n\left\{\mathcal{E}_{0,n}(t) - \mathcal{E}_{s,n}(t)\right\} - V_m\left\{\mathcal{E}_{0,m}(t) - \mathcal{E}_{s,m}(t)\right\}\right]\Bigg|_{t=0}^{2\pi}\\
&\qquad - \int_0^{2\pi} g(e^{it})\ \operatorname{Tr}\left[V_n\left\{\mathcal{E}_{0,n}(dt) - \mathcal{E}_{s,n}(dt)\right\} - V_m\left\{\mathcal{E}_{0,m}(dt) - \mathcal{E}_{s,m}(dt)\right\}\right]\Bigg] ds\\
&= -\int_0^1 ds \int_0^{2\pi} g(e^{it})\ \operatorname{Tr}\left[V_n\left\{\mathcal{E}_{0,n}(dt) - \mathcal{E}_{s,n}(dt)\right\} - V_m\left\{\mathcal{E}_{0,m}(dt) - \mathcal{E}_{s,m}(dt)\right\}\right]\\
&= \int_0^1 ds\ \operatorname{Tr}\left[V_n\left\{g(N_{s,n}) - g(N_{0,n})\right\} - V_m\left\{g(N_{s,m}) - g(N_{0,m})\right\}\right]\\
&= \int_0^1 ds\ \operatorname{Tr}\Bigg[V_n\bigg\{\left\{g(N_{s,n}) - g(N_s)\right\} - \left\{g(N_{0,n}) - g(N_0)\right\}\bigg\}\\
&\qquad - V_m\bigg\{\left\{g(N_{s,m}) - g(N_s)\right\} - \left\{g(N_{0,m}) - g(N_0)\right\}\bigg\} + (V_n - V_m)\left\{g(N_s) - g(N_0)\right\}\Bigg].
\end{aligned} \tag{3.27}$$

On the other hand using Theorem 3.2.2 and using trace properties we obtain for $s \in [0, 1]$ that

$$\begin{aligned}
&\left|\operatorname{Tr}\left[V_n\{g(N_{s,n}) - g(N_s)\}\right]\right| = \left|\operatorname{Tr}\left[V_n P_n\{g(N_s) - g(N_{s,n})\}P_n\right]\right|\\
&\leq \|V_n\|_2\ \left\|P_n\left\{g(N_s) - g(N_{s,n})\right\}P_n\right\|_2 \leq \|V\|_2\ \left\|P_n\left\{g(N_s)P_n - P_n\ g(N_{s,n})\right\}P_n\right\|_2\\
&\leq \|V\|_2\ \left\|g(N_s)P_n - P_n\ g(N_{s,n})\right\|_2 \leq \|f\|_\infty \|V\|_2\ \left\|N_sP_n - P_nN_{s,n}\right\|_2
\end{aligned}$$

$$= \|f\|_\infty \|V\|_2 \left\|P_n^\perp N_s P_n\right\|_2 \le \|f\|_\infty \|V\|_2 \left(\left\|P_n^\perp N_0 P_n\right\|_2 + \left\|P_n^\perp V\right\|_2\right). \tag{3.28}$$

Similarly, by repeating the above calculations we also obtain

$$\begin{aligned}\left|\mathrm{Tr}\left[(V_n - V_m)\{g(N_s) - g(N_0)\}\right]\right| &\le \|f\|_\infty \|V\|_2 \left\|V_n - V_m\right\|_2 \\ &\le \|f\|_\infty \|V\|_2 \left(\left\|P_n^\perp V\right\|_2 + \left\|V P_n^\perp\right\|_2 + \left\|P_m^\perp V\right\|_2 + \left\|V P_m^\perp\right\|_2\right). \end{aligned}\tag{3.29}$$

Now combining (3.27), (4.9) and (3.29) we get

$$\begin{aligned}&\left|\int_{\mathbb{T}} f(z)\{\eta_n(z) - \eta_m(z)\}dz\right| \\ &\le \int_0^1 ds \left|\mathrm{Tr}\left[V_n\left\{\left\{g(N_{s,n}) - g(N_s)\right\} - \left\{g(N_{0,n}) - g(N_0)\right\}\right\}\right.\right. \\ &\qquad \left.\left. - V_m\left\{\left\{g(N_{s,m}) - g(N_s)\right\} - \left\{g(N_{0,m}) - g(N_0)\right\}\right\} + (V_n - V_m)\left\{g(N_s) - g(N_0)\right\}\right]\right| \\ &\le K_{m,n} \|f\|_\infty \|V\|_2, \end{aligned}\tag{3.30}$$

where

$$\begin{aligned}K_{m,n} = &\left\{2\left(\left\|P_n^\perp N_0 P_n\right\|_2 + \left\|P_n^\perp V\right\|_2\right) + 2\left(\left\|P_m^\perp N_0 P_m\right\|_2 + \left\|P_m^\perp V\right\|_2\right)\right. \\ &\left. + \left(\left\|P_n^\perp V\right\|_2 + \left\|V P_n^\perp\right\|_2 + \left\|P_m^\perp V\right\|_2 + \left\|V P_m^\perp\right\|_2\right)\right\}.\end{aligned}$$

Therefore using Lemma 3.2.1 and the above estimate (3.30) we conclude

$$\begin{aligned}\left\|[\eta_n] - [\eta_m]\right\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} = \left\|[\eta_n - \eta_m]\right\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} &= \sup_{f \in \mathcal{P}(\mathbb{T});\ \|f\|_\infty \le 1} \left|\int_{\mathbb{T}} f(z)\{\eta_n(z) - \eta_m(z)\}dz\right| \\ &\le K_{m,n} \|V\|_2 \longrightarrow 0 \quad \text{as} \quad m, n \longrightarrow \infty,\end{aligned}$$

by using Theorem 3.4.3 and hence $\left\{[\eta_n]\right\}$ is a Cauchy sequence in $L^1(\mathbb{T})/H^1(\mathbb{T})$. Consequently, there exists a $\eta \in L^1(\mathbb{T})$ such that $\left\{[\eta_n]\right\}$ converges to $[\eta]$ in $L^1(\mathbb{T})/H^1(\mathbb{T})$-norm, that is

$$\lim_{n \longrightarrow \infty} \left\|[\eta_n] - [\eta]\right\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} = 0,$$

which in particular implies that

$$\lim_{n \longrightarrow \infty} \int_{\mathbb{T}} p(z)\eta_n(z)dz = \int_{\mathbb{T}} p(z)\eta(z)dz \tag{3.31}$$

for all complex polynomials $p(\cdot)$. Therefore combining (3.24) and (3.31) we get

$$\operatorname{Tr}\left\{p(N) - p(N_0) - \frac{d}{ds}\bigg|_{s=0} p(N_s)\right\} = \lim_{n\to\infty}\int_{\mathbb{T}} p''(z)\eta_n(z)dz = \int_{\mathbb{T}} p''(z)\eta(z)dz.$$

Furthermore, the equation (3.26) yields

$$\big\|[\eta]\big\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} \leq \frac{1}{2}\,\|V\|_2^2,$$

which by applying the definition of the $L^1(\mathbb{T})/H^1(\mathbb{T})$- norm, for every $\epsilon > 0$, there is a function $\eta \in L^1(\mathbb{T})$ such that

$$\big\|\eta\big\|_{L^1(\mathbb{T})} \leq \left(\frac{1}{2}+\epsilon\right)\,\|V\|_2^2.$$

This completes the proof. □

Our next aim is to extend the class of functions for which the trace formula (3.22) holds. For that we need the following lemma. The proof of the following lemma is similar to the proof of Lemma 2.4.2, so we state it without proof.

Lemma 3.5.2. *Let T and T_0 be two contractions in a separable infinite dimensional Hilbert space $\mathcal{H}$ and $f(z) = \sum_{k=0}^{\infty} a_k z^k \in \mathcal{F}_2^+(\mathbb{T})$. Let $T_s = T_0 + s(T - T_0)$, $s \in [0,1]$, then*

$$\frac{d}{ds}\bigg|_{s=0}\left(\sum_{k=0}^{\infty} a_k (T_s)^k\right) = \sum_{k=0}^{\infty} a_k\,\frac{d}{ds}\bigg|_{s=0}(T_s)^k. \tag{3.32}$$

Now we are in a position to prove our main result in this section.

Theorem 3.5.3. *Let N be a contraction and N_0 be a normal contraction in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $V = N - N_0 \in \mathcal{B}_2(\mathcal{H})$. Denote $N_s = N_0 + sV$, $s \in [0,1]$. Then for any $\Phi \in \mathcal{F}_2^+(\mathbb{T})$, $\left\{\Phi(N) - \Phi(N_0) - \frac{d}{ds}\Big|_{s=0}\Phi(N_s)\right\} \in \mathcal{B}_1(\mathcal{H})$ and there exists an $L^1(\mathbb{T})$-function η (unique up to an analytic term) such that*

$$\operatorname{Tr}\left\{\Phi(N) - \Phi(N_0) - \frac{d}{ds}\bigg|_{s=0}\{\Phi(N_s)\}\right\} = \int_{\mathbb{T}} \Phi''(z)\eta(z)dz. \tag{3.33}$$

Furthermore, for every given $\epsilon > 0$, we choose the function η satisfying (3.33) in such a way so that

$$\|\eta\|_{L^1(\mathbb{T})} \leq \left(\frac{1}{2}+\epsilon\right)\,\|V\|_2^2.$$

Proof. Let $\Phi(z) = \sum_{n=0}^{\infty} a_n z^n \in \mathcal{F}_2^+(\mathbb{T})$. Then by Lemma 3.5.2, we get

$$\begin{aligned}\Phi(N) - \Phi(N_0) - \frac{d}{ds}\Big|_{s=0} \Phi(N_s) &= \sum_{n=0}^{\infty} a_n N^n - \sum_{n=0}^{\infty} a_n N_0^n - \frac{d}{ds}\Big|_{s=0} \left(\sum_{n=0}^{\infty} a_n N_s^n \right) \\ &= \sum_{n=0}^{\infty} a_n \left[N^n - N_0^n - \frac{d}{ds}\Big|_{s=0} N_s^n \right]. \end{aligned} \tag{3.34}$$

By Theorem 3.5.3, we conclude that $\left\{ N^n - N_0^n - \frac{d}{ds}\Big|_{s=0} N_s^n \right\} \in \mathcal{B}_1(\mathcal{H})$ and the following trace norm estimate

$$\begin{aligned}\left\| N^n - N_0^n - \frac{d}{ds}\Big|_{s=0} N_s^n \right\|_1 &= \left\| N^n - N_0^n - \sum_{j=0}^{n-1} N_0^{n-j-1} V N_0^j \right\|_1 \\ &= \left\| \sum_{j=0}^{n-1} (N^{n-j-1} - N_0^{n-j-1}) V N_0^j \right\|_1 \\ &\leq \left\| \sum_{j=1}^{n-1} \sum_{k=0}^{n-j-2} N^{n-j-k-2} V N_0^k V N_0^j \right\|_1 \\ &\leq \sum_{j=1}^{n-1} \sum_{k=0}^{n-j-2} \|V\|_2^2 \leq \frac{n(n-1)}{2} \|V\|_2^2 \end{aligned}$$

implies

$$\sum_{n=0}^{\infty} |a_n| \left\| N^n - N_0^n - \frac{d}{ds}\Big|_{s=0} N_s^n \right\|_1 \leq \sum_{n=0}^{\infty} |a_n| \frac{n(n-1)}{2} \|V\|_2^2 < \infty. \tag{3.35}$$

Therefore the series in (3.34) converges in trace norm and hence $\left\{ \Phi(N) - \Phi(N_0) - \frac{d}{ds}\Big|_{s=0} \Phi(N_s) \right\}$ is a trace class operator and furthermore

$$\operatorname{Tr} \left\{ \Phi(N) - \Phi(N_0) - \frac{d}{ds}\Big|_{s=0} \Phi(N_s) \right\} = \sum_{n=0}^{\infty} a_n \operatorname{Tr} \left\{ N^n - N_0^n - \frac{d}{ds}\Big|_{s=0} N_s^n \right\}. \tag{3.36}$$

Therefore by applying Theorem 3.5.1, the above equation (3.36) yields

$$\operatorname{Tr} \left\{ \Phi(N) - \Phi(N_0) - \frac{d}{ds}\Big|_{s=0} \Phi(N_s) \right\} = \sum_{n=2}^{\infty} \int_{\mathbb{T}} \left\{ n(n-1) a_n z^{n-2} \right\} \eta(z) dz = \int_{\mathbb{T}} \Phi''(z) \eta(z) dz,$$

where at the last equality, we have used Fubini's theorem and the function η as in Theorem 3.5.1 satisfying the equation (3.23). This completes the proof. □

Corollary 3.5.1. *If U and U_0 are two unitary operators in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$. Denote $U_s = U_0 + sV$, $s \in [0,1]$, and $U = U_1$.*

Then there exists a $L^1(\mathbb{T})$-function η (unique up to an analytic term) and satisfying the equation (3.23) such that, for any $z \in \mathbb{C}$ with $|z| > 1$,

$$\operatorname{Tr}\left\{(U-z)^{-1} - (U_0-z)^{-1} - \frac{d}{ds}\Big|_{s=0}(U_s-z)^{-1}\right\} = \int_{\mathbb{T}} \frac{d^2}{dw^2}\Big\{(w-z)^{-1}\Big\}\eta(w)dw.$$

3.6 Trace formula for contractions

In this section we prove the trace formula for class of pairs of contractions (T, T_0) such that $T - T_0 \in \mathcal{B}_2(\mathcal{H})$ using the Schäffer matrix unitary dilation (see Chapter 1, Section 1.6). The following lemma is essential to prove our main results in this section.

Lemma 3.6.1. *Let T and T_0 be two contractions in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $V = T - T_0 \in \mathcal{B}_2(\mathcal{H})$. Let $T_s = T_0 + sV$, $s \in [0,1]$. Then for any complex polynomial $p(\cdot)$, $\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0}\{p(T_s)\}\right\} \in \mathcal{B}_1(\mathcal{H})$ and*

$$\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0}\{p(T_s)\}\right\} = \lim_{t\to 0}\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{p(T_t) - p(T_0)}{t}\right\}. \tag{3.37}$$

Proof. It will be sufficient to prove the theorem for $p(z) = z^r$. Note that for $r = 0$ or 1, both sides of (3.37) are identically zero. Now by using similar kind of expressions as in (3.6) and (3.7), we conclude $\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0} p(T_s)\right\}, \left\{p(T) - p(T_0) - \frac{p(T_t)-p(T_0)}{t}\right\} \in \mathcal{B}_1(\mathcal{H})$ for $t \in [0,1]$. Furthermore,

$$\begin{aligned}
&\left\| \left\{p(T) - p(T_0) - \frac{p(T_t) - p(T_0)}{t}\right\} - \left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0} p(T_s)\right\} \right\|_1 \\
&= \left\| \left\{T^r - T_0^r - \frac{T_t^r - T_0^r}{t}\right\} - \left\{T^r - T_0^r - \sum_{j=0}^{r-1} T_0^{r-j-1} V T_0^j\right\} \right\|_1 \\
&= \left\| \sum_{j=0}^{r-1} T_t^{r-j-1} V T_0^j - \sum_{j=0}^{r-1} T_0^{r-j-1} V T_0^j \right\|_1 = \left\| \sum_{j=0}^{r-2}\sum_{k=0}^{r-j-2} T_t^{r-j-k-2} t V T_0^k V T_0^j \right\|_1 \\
&\leq \ |t| \sum_{j=0}^{r-2}\sum_{k=0}^{r-j-2} \|T_t^{r-j-k-2} V T_0^k\|_2 \|V T_0^j\|_2 \leq \ |t| \sum_{j=0}^{r-2}\sum_{k=0}^{r-j-2} \|V\|_2^2 \to 0 \text{ as } t \to 0,
\end{aligned}$$

and hence (3.37) follows. This completes the proof. □

Motivated from the work of Marcantognini and Morán [40] we have the following one of the main result in this section.

Theorem 3.6.2. *Let T and T_0 be two contractions in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that*

(i) $T - T_0 \in \mathcal{B}_2(\mathcal{H})$, (ii) $\dim\ker(T_0) = \dim\ker(T_0^*)$, and (iii) $D_{T_0} \in \mathcal{B}_2(\mathcal{H})$. Denote $T_s = T_0 + s(T - T_0)$, $s \in [0,1]$. Then for any complex polynomial $p(\cdot)$, $\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0}\{p(T_s)\}\right\} \in \mathcal{B}_1(\mathcal{H})$ and there exists an $L^1(\mathbb{T})$-function η (unique up to an analytic term) such that

$$\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0}\{p(T_s)\}\right\} = \int_{\mathbb{T}} p''(z)\eta(z)dz. \tag{3.38}$$

Moreover, the function η satisfying (3.38) also satisfies the equation (3.23).

Proof. Let U_{T_0} be the minimal Schäffer matrix unitary dilation of T_0 (see Chapter 1, Section 1.6) on the minimal dilation space $\mathcal{K} := l^2_{\mathbb{N}}(\mathcal{D}_{T_0}) \oplus \mathcal{H} \oplus l^2_{\mathbb{N}}(\mathcal{D}_{T_0^*})$ and we have the same block matrix representation of U_{T_0} as in (1.12) on $\mathcal{K}$. Let $T_0 = V_{T_0}|T_0|$ be the polar decomposition of T_0, so that $|T_0| = (T_0^*T_0)^{1/2}$ and V_{T_0} is an isometry from $\overline{\operatorname{Ran}(T_0^*)}$ onto $\overline{\operatorname{Ran}(T_0)}$. Since $\dim\ker(T_0) = \dim\ker(T_0^*)$, then we can extend V_{T_0} to a unitary operator on the full space $\mathcal{H}$. Now onward we assume V_{T_0} is a unitary operator on $\mathcal{H}$ such that $T_0 = V_{T_0}|T_0|$. Next we note that

$$V_{T_0}D_{T_0} = D_{T_0^*}V_{T_0} \text{ and } V_{T_0} - T_0 = V_{T_0}(1 - |T_0|) = V_{T_0}(1 - T_0^*T_0)(1 + |T_0|)^{-1}. \tag{3.39}$$

Now we extend T to a contraction U_T on $\mathcal{K}$ be setting

$$U_{T} = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdot^{\cdot^{\cdot}} \\ \cdots & 0 & 0 & I & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & -V_{T_0}^* & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & \boxed{T} & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & 0 & I & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & 0 & 0 & I & \cdots \\ \cdot^{\cdot^{\cdot}} & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \tag{3.40}$$

Note that in the above block matrix representation (3.40) of U_T, the (i,j)-th entries $U_{T}(i,j)$ of U_{T} are given by

$$U_{T}(0,0) = T,\ U_{T}(-1,0) = 0,\ U_{T}(-1,1) = -V_{T_0}^*,\ U_{T}(0,1) = 0,\ U_{T}(j,j+1) = I$$

for $j \neq 0, -1$, while all the remaining entries are equal to zero. Therefore we have

$$T^n = \tilde{P}_{\mathcal{H}} U_T^n|_{\mathcal{H}} \quad \text{and} \quad T_0^n = \tilde{P}_{\mathcal{H}} U_{T_0}^n|_{\mathcal{H}} \quad \text{for} \quad n \geq 1,$$

where $\tilde{P}_{\mathcal{H}}$ is the orthogonal projection of $\mathcal{K}$ onto $\mathcal{H}$. By hypothesis (i), (iii) and using the relation (3.39) we conclude $U_T - U_{T_0} \in \mathcal{B}_2(\mathcal{K})$. Denote $U_{t,T} = (1-t)U_{T_0} + tU_T = U_{T_0} + t(U_T - U_{T_0})$ for $t \in [0,1]$. Note that $p(U_T)$ and $p(U_{T_0})$ are upper triangular matrices with the only nonzero diagonal entries $p(T)$ and $p(T_0)$. Thus $\left\{p(U_T) - p(U_{T_0}) - \frac{p(U_{t,T}) - p(U_{T_0})}{t}\right\}$ is an upper triangular matrix with the only nonzero diagonal entry $\left\{p(T) - p(T_0) - \frac{p(T_t) - p(T_0)}{t}\right\}$ and hence

$$\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{p(T_t) - p(T_0)}{t}\right\} = \operatorname{Tr}\left\{p(U_T) - p(U_{T_0}) - \frac{p(U_{t,T}) - p(U_{T_0})}{t}\right\} \quad \text{for} \quad t \in [0,1]. \tag{3.41}$$

Therefore by applying Lemma 3.6.1 corresponding to pair of contractions (T, T_0) and (U_T, U_{T_0}) and using (3.41) we get

$$\begin{aligned}
\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} p(T_s)\right\} &= \lim_{t\to 0} \operatorname{Tr}\left\{p(T) - p(T_0) - \frac{p(T_t) - p(T_0)}{t}\right\} \\
= \lim_{t\to 0} \operatorname{Tr}\left\{p(U_T) - p(U_{T_0}) - \frac{p(U_{t,T}) - p(U_{T_0})}{t}\right\} &= \operatorname{Tr}\left\{p(U_T) - p(U_{T_0}) - \frac{d}{ds}\bigg|_{s=0} p(U_{s,T})\right\},
\end{aligned}$$

which by applying Theorem 3.5.1 corresponding to the pair (U_T, U_{T_0}) we conclude that there exists an $L^1(\mathbb{T})$-function η (unique up to an analytic term) satisfying (3.23) such that

$$\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} \{p(T_s)\}\right\} = \int_{\mathbb{T}} p''(z)\eta(z)dz.$$

This completes the proof. □

The following theorem is the second main result in this section in which we prove the trace formula for a class of pairs of contractions different from the class mentioned in Theorem 3.6.2.

Theorem 3.6.3. *Let T and T_0 be two contractions in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $U_T - U_{T_0} \in \mathcal{B}_2(l^2_{\mathbb{Z}}(\mathcal{H}))$. Denote $T_s = T_0 + s(T - T_0)$, $s \in [0,1]$. Then for any complex polynomial $p(\cdot)$, $\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0} \{p(T_s)\}\right\} \in \mathcal{B}_1(\mathcal{H})$ and there exists an $L^1(\mathbb{T})$-function η (unique up to an analytic term) such that*

$$\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} \{p(T_s)\}\right\} = \int_{\mathbb{T}} p''(z)\eta(z)dz. \tag{3.42}$$

Moreover, the function η satisfying (3.42) also satisfies the equation (3.23).

Proof. Note that U_T and U_{T_0} are the Schäffer matrix unitary dilation of T and T_0 respectively on the same Hilbert space $l^2_{\mathbb{Z}}(\mathcal{H})$ (see (1.12)), that is

$$T^n = P_{\mathcal{H}} U_T^n|_{\mathcal{H}} \quad \text{and} \quad T_0^n = P_{\mathcal{H}} U_{T_0}^n|_{\mathcal{H}} \quad \text{for} \quad n \geq 1, \tag{3.43}$$

where $P_{\mathcal{H}}$ as in (1.11). Since $U_{_T} - U_{_{T_0}} \in \mathcal{B}_2(l^2_{\mathbb{Z}}(\mathcal{H}))$, then from (3.43) we conclude $T - T_0 \in \mathcal{B}_2(\mathcal{H})$. Denote $U_{t,T} = (1-t)U_{T_0} + tU_T = U_{T_0} + t(U_T - U_{T_0})$ for $t \in [0,1]$. Then by the similar argument as in Theorem 3.6.2 we conclude the theorem. □

Remark 3.6.4. *In a similar spirit as in Theorem 3.5.3, we also prove Theorem 3.6.3 corresponding to the class $\mathcal{F}_2^+(\mathbb{T})$.*

3.7 Trace formula for self-adjoint operators

In this section, motivated from the work of Neidhardt in [42, Section 3] we prove the trace formula for a pair of self-adjoint operators H_0 and H_1 on an infinite-dimensional Hilbert space $\mathcal{H}$ such that the difference $(H_1 - i)^{-1} - (H_0 - i)^{-1} \in \mathcal{B}_2(\mathcal{H})$ via Cayley transform.

Let H and H_0 be two arbitrary self-adjoint operators in $\mathcal{H}$ such that $\text{Dom}(H) = \text{Dom}(H_0)$, and let

$$U = (i - H)(i + H)^{-1} \quad \text{and} \quad U_0 = (i - H_0)(i + H_0)^{-1} \tag{3.44}$$

be the corresponding unitary operators obtained via the Cayley transform of H and H_0 respectively (see Chapter 1). Let $\psi(\lambda) = \phi\left(\frac{i-\lambda}{i+\lambda}\right) \in \mathcal{F}_2^+(\mathbb{R})$ for some $\phi \in \mathcal{F}_2^+(\mathbb{T})$, $U_s = (1-s)U_0 + sU$, and $H_s = sH_0 + (1-s)H$ for $s \in [0,1]$. Then it is easy to observe that

$$\psi(H) = \phi(U), \ \psi(H_0) = \phi(U_0), \ \text{and} \ \psi(W_s) = \phi(U_s),$$

where

$$W_s = \Big((H+i)(H_s+i)^{-1}(H_0+i) - i\Big),$$

and hence we have the following operator equality

$$\psi(H) - \psi(H_0) - \frac{d}{ds}\Big|_{s=0} \psi(W_s) = \ \phi(U) - \phi(U_0) - \frac{d}{ds}\Big|_{s=0} \phi(U_s). \tag{3.45}$$

In the following, we denote $R_z = (H - z)^{-1}$ for $z \in \mathbb{C}$ as the resolvent operator corresponding to an unbounded self-adjoint operator H and $\rho(H)$ is the associated resolvent set. Moreover, we also denote $\mathrm{Dom}(H)$ as the domain of definition of the self-adjoint operator H (possibly unbounded). The following is the main result in this section.

Theorem 3.7.1. *Let H and H_0 be two self-adjoint operators in a separable infinite dimensional Hilbert space $\mathcal{H}$ such that $\mathrm{Dom}(H) = \mathrm{Dom}(H_0)$ and $R_z - R_z^0 \in \mathcal{B}_2(\mathcal{H})$ for some $z \in \rho(H) \cap \rho(H_0)$. Let*

$$W_s = \Big((H+i)(H_s+i)^{-1}(H_0+i) - i\Big),$$

where $H_s = sH_0 + (1-s)H,\ s \in [0,1]$. Then there exists a measurable function $\xi : \mathbb{R} \to \mathbb{C}$ obeying $(1+\lambda^2)^{-1}\xi \in L^1(\mathbb{R})$ such that

$$\mathrm{Tr}\left\{\psi(H) - \psi(H_0) - \frac{d}{ds}\Big|_{s=0}\psi(W_s)\right\} = \int_{-\infty}^{\infty} \frac{d}{d\lambda}\Big\{(1+\lambda^2)\psi'(\lambda)\Big\}\ \xi(\lambda)\ d\lambda \tag{3.46}$$

for each $\psi \in \mathcal{F}_2^+(\mathbb{R})$. In particular, for all $z \in \mathbb{C}$ with $\mathrm{Im}(z) < 0$,

$$\mathrm{Tr}\left\{(H-z)^{-1} - (H_0-z)^{-1} - \frac{i+H_0}{H_0-z}\ M\ \frac{i+H_0}{H_0-z}\right\} = \int_{-\infty}^{\infty} \frac{2(1+\lambda z)}{(\lambda - z)^3}\ \xi(\lambda)\ d\lambda, \tag{3.47}$$

where $M = R_{-i} - R_{-i}^0$.

Proof. Let U and U_0 be as in (3.44). Since $R_z - R_z^0 \in \mathcal{B}_2(\mathcal{H})$, then it immediately follows that $U - U_0 \in \mathcal{B}_2(\mathcal{H})$. Therefore using the above identity (3.45) and using Theorem 3.5.3 we conclude that there exists an $L^1(\mathbb{T})$-function η (unique up to an analytic term) such that

$$\begin{aligned}
&\mathrm{Tr}\left\{\psi(H) - \psi(H_0) - \frac{d}{ds}\Big|_{s=0}\psi\left(W_s\right)\right\}\\
&= \mathrm{Tr}\left\{\phi(U) - \phi(U_0) - \frac{d}{ds}\Big|_{s=0}\phi(U_s)\right\} = \int_{\mathbb{T}} \phi''(z)\eta(z)dz\\
&= \int_{\mathbb{T}} \phi''(z)\left(\eta(z) - \frac{z}{2\pi i}\int_{\mathbb{T}}\frac{\eta(\omega)}{\omega^2}d\omega\right)dz = \int_{\mathbb{T}} \phi''(z)\Gamma(z)dz,
\end{aligned} \tag{3.48}$$

where

$$\Gamma(z) = \eta(z) - \frac{z}{2\pi i}\int_{\mathbb{T}}\frac{\eta(\omega)}{\omega^2}d\omega, \quad z \in \mathbb{T}.$$

Next by using change of variables $z = e^{it}$, performing integration by-parts and using the fact that $\int_0^{2\pi} e^{-is}\Gamma(e^{is})ds = 0$ we get

$$\mathrm{Tr}\left\{\psi(H) - \psi(H_0) - \frac{d}{ds}\Big|_{s=0}\psi\left(W_s\right)\right\}$$

$$= \int_0^{2\pi} \frac{d^2}{dt^2}\{\phi(e^{it})\}\left(-ie^{-it}\right)\Gamma(e^{it})dt - \int_0^{2\pi} \frac{d}{dt}\{\phi(e^{it})\}e^{-it}\Gamma(e^{it})dt \tag{3.49}$$

$$= \int_0^{2\pi} \frac{d^2}{dt^2}\{\phi(e^{it})\}\left[\left(-ie^{-it}\right)\Gamma(e^{it}) + \left(\int_0^t e^{-is}\Gamma(e^{is})ds\right)\right]dt$$

$$= \int_0^{2\pi} \frac{d^2}{dt^2}\{\phi(e^{it})\}\ \tilde{\eta}(e^{it})\ dt, \tag{3.50}$$

where

$$\tilde{\eta}(e^{it}) = \left(-ie^{-it}\right)\Gamma(e^{it}) + \left(\int_0^t e^{-is}\Gamma(e^{is})ds\right),\ t \in [0, 2\pi].$$

Clearly $\tilde{\eta} \in L^1([0, 2\pi])$ and again by using change of variables $e^{it} = \dfrac{i-\lambda}{i+\lambda}$, from (3.49) we conclude

$$\text{Tr}\left\{\psi(H) - \psi(H_0) - \frac{d}{ds}\Big|_{s=0}\psi\left(W_s\right)\right\} = \int_{-\infty}^{\infty} \frac{d}{d\lambda}\left\{(1+\lambda^2)\psi'(\lambda)\right\}\xi(\lambda)\ d\lambda,$$

where $\xi(\lambda) = \dfrac{1}{2}\tilde{\eta}\left(\dfrac{i-\lambda}{i+\lambda}\right), \lambda \in \mathbb{R}$, and moreover

$$\int_{-\infty}^{\infty} \frac{|\xi(\lambda)|}{1+\lambda^2}\ d\lambda = \frac{1}{4}\int_0^{2\pi} |\tilde{\eta}(e^{it})|\ dt < \infty.$$

Next, we denote $\tau = \frac{i-z}{i+z}$ for $z \in \mathbb{C}$ with $\text{Im}(z) < 0$. Then it is easy to observe that $|\tau| > 1$. Now consider $\psi(\lambda) = (\lambda - z)^{-1}$, $\lambda \in \mathbb{R}$, and $\phi(w) = \dfrac{i(1+\tau)^2}{2}\left[\dfrac{1}{1+\tau} + \dfrac{1}{w-\tau}\right]$, $w \in \mathbb{T}$. Then it is easy to conclude that $\psi(\lambda) = \phi\left(\dfrac{i-\lambda}{i+\lambda}\right)$, $\phi \in \mathcal{F}_2^+(\mathbb{T})$ and hence $\psi \in \mathcal{F}_2^+(\mathbb{R})$. Therefore by applying (3.46) corresponding to ψ we get

$$\text{Tr}\left\{(H-z)^{-1} - (H_0 - z)^{-1} - \frac{d}{ds}\Big|_{s=0}(W_s - z)^{-1}\right\} = \int_{-\infty}^{\infty} \frac{2(1+\lambda z)}{(\lambda - z)^3}\ \xi(\lambda)\ d\lambda. \tag{3.51}$$

On the other hand the equality $\phi(U_0) = \psi(H_0)$ yields that

$$(U_0 - \tau)^{-1} = \frac{i}{2}(i+z)\frac{i+H_0}{H_0 - z},$$

and hence

$$\frac{d}{ds}\Big|_{s=0}(W_s - z)^{-1} = \frac{i(1+\tau)^2}{2}\ \frac{d}{ds}\Big|_{s=0}(U_s - \tau)^{-1}$$

$$= -2i\ \frac{i(1+\tau)^2}{2}(U_0 - \tau)^{-1}(R_{-i} - R_{-i}^0)(U_0 - \tau)^{-1}$$

$$= \frac{i+H_0}{z-H_0}\ M\ \frac{i+H_0}{z-H_0}, \tag{3.52}$$

where $M = R_{-i} - R_{-i}^0$. Therefore combining equations (3.51) and (3.52) we get (3.47). This completes the proof. □

Remark 3.7.2. *It is important to note that even though the formulas* (3.46) *and* (3.47) *are look like similar to the formulas (3.12) and (3.11) respectively obtained in [42, Theorem 3.2], but they are actually different since our path* $W_s = \Big((H+i)(H_s+i)^{-1}(H_0+i)-i\Big)$ *is not exactly same as the path considered by Neidhardt in [42, Theorem 3.2]. In other words, we have obtained the path* W_s *by considering the Cayley transformation on the linear path associated to the pair* (U, U_0) *whereas Neidhardt obtained the required path by considering the Cayley transformation on the multiplicative path associated to the pair* (U, U_0)*. Furthermore, the path* W_s *is closer to the path considered by Koplienko [31].*

3.8 Trace formula for maximal dissipative operators

In this section, our aim is to obtain the Koplienko trace formula for a pair of maximal dissipative operators from the existing Koplienko trace formula (3.3) corresponding to a pair of contractions (T, T_0) such that $T - T_0 \in \mathcal{B}_2(\mathcal{H})$. In this connection, it is worth mentioning a paper by Malamud, Neidhardt and Peller [39], where an analogous study of Krein's trace formula for a pair of maximal dissipative operators was achieved. Recall that the Cayley transform of a maximal dissipative operator L is defined by

$$T = (i - L)(i + L)^{-1}. \tag{3.53}$$

It is well known that T is a contraction. Moreover, a contraction T is the Cayley transform of a maximal dissipative operator L if and only if -1 is not an eigenvalue of T (see Lemma 1.2.12). Now we have the following main theorem in this section.

Theorem 3.8.1. *Let* L *and* L_0 *be two maximal dissipative operators in a separable infinite dimensional Hilbert space* $\mathcal{H}$ *such that* $\mathrm{Dom}(L) = \mathrm{Dom}(L_0)$ *and* $(L+i)^{-1} - (L_0+i)^{-1} \in \mathcal{B}_2(\mathcal{H})$*. Let*

$$Q_s = \Big((L+i)(L_s+i)^{-1}(L_0+i) - i\Big),$$

where $L_s = sL_0 + (1-s)L$, $s \in [0,1]$*. Then there exists a measurable function* $\xi : \mathbb{R} \to \mathbb{C}$ *obeying* $(1+\lambda^2)^{-1}\xi \in L^1(\mathbb{R})$ *such that*

$$\mathrm{Tr}\left\{\psi(L) - \psi(L_0) - \frac{d}{ds}\Big|_{s=0}\psi(Q_s)\right\} = \int_{-\infty}^{\infty} \frac{d}{d\lambda}\Big\{(1+\lambda^2)\psi'(\lambda)\Big\}\, \xi(\lambda)\, d\lambda \tag{3.54}$$

for each $\psi \in \mathcal{F}_{\mathbb{R}}$*.*

Proof. Let T and T_0 be the Cayley transform of L and L_0 respectively, that is

$$T = (i - L)(i + L)^{-1} \text{ and } T_0 = (i - L_0)(i + L_0)^{-1}.$$

Consequently,

$$L = i(1 - T)(1 + T)^{-1} \text{ and } L_0 = i(1 - T_0)(1 + T_0)^{-1}.$$

It is easy to observe that $(i - Q_s)(i + Q_s)^{-1} = T_s$. Let $\psi \in \mathcal{F}_{\mathbb{R}}$. Then there exists $\phi \in \mathcal{A}_{\mathbb{T}}$ such that $\psi(\lambda) = \phi\left(\frac{i-\lambda}{i+\lambda}\right)$ and hence $\psi(L) = \phi(T)$, $\psi(L_0) = \phi(T_0)$ and $\psi(Q_s) = \phi(T_s)$. Therefore by similar kind of argument as in Theorem 3.7.1 and using Theorem 3.1.1 we conclude that there exists a measurable function $\xi : \mathbb{R} \to \mathbb{C}$ obeying $(1 + \lambda^2)^{-1}\xi \in L^1(\mathbb{R})$ such that

$$\operatorname{Tr}\left\{\psi(L) - \psi(L_0) - \frac{d}{ds}\Big|_{s=0}\psi(Q_s)\right\} = \int_{-\infty}^{\infty} \frac{d}{d\lambda}\left\{(1 + \lambda^2)\psi'(\lambda)\right\} \xi(\lambda)\, d\lambda.$$

This completes the proof. □

3.9 Extension of Koplienko-Neidhardt trace formula

In this section, we deal with the extension of the Koplienko-Neidhardt trace formula in the following sense: Neidhardt obtained the formula (2.4) corresponding to the pair (U_0, A), where U_0 is a unitary operator on $\mathcal{H}$ and $A = A^* \in \mathcal{B}_2(\mathcal{H})$. In this regard, the following theorem deals with the formula (2.4) corresponding to the pair (T_0, A), where $T_0 = N_0 + V$ is a contraction on $\mathcal{H}$ such that N_0 is a bounded normal operator on $\mathcal{H}$, $V \in \mathcal{B}_2(\mathcal{H})$ and $A = A^* \in \mathcal{B}_2(\mathcal{H})$. We use finite dimensional approximation method as earlier to prove our result.

Theorem 3.9.1. *Let $T_0 = N_0 + V$ be a contraction in an infinite dimensional separable Hilbert space $\mathcal{H}$ such that $N_0^* N_0 = N_0 N_0^*$ and $V \in \mathcal{B}_2(\mathcal{H})$. Let $A = A^* \in \mathcal{B}_2(\mathcal{H})$. Denote $T_s = e^{isA}T_0,\ s \in [0, 1]$, and $T = T_1$. Then for any complex polynomial $p(\cdot)$,*

$$\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0} \{p(T_s)\}\right\} \in \mathcal{B}_1(\mathcal{H})$$

and there exists an $L^1(\mathbb{T})$-function $\tilde{\eta}$ (unique up to an analytic term) such that

$$\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\Big|_{s=0} \{p(T_s)\}\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\left(p(e^{it})\right)\tilde{\eta}(t)dt. \tag{3.55}$$

Moreover, for every given $\epsilon > 0$, we choose the function $\tilde{\eta}$ satisfying (3.55) in such a way so that

$$\|\tilde{\eta}\|_{L^1(\mathbb{T})} \leq (\frac{1}{2} + \epsilon)\ \|A\|_2^2. \tag{3.56}$$

Proof. Using Theorem 3.4.6 and Theorem 3.3.4, we have that

$$\begin{aligned}\operatorname{Tr}\left\{p(T)-p(T_0)-\frac{d}{ds}\Big|_{s=0}p(T_s)\right\} &= \lim_{n\to\infty}\operatorname{Tr}\left[P_n\left\{p(T_n)-p(T_{0,n})-\frac{d}{ds}\Big|_{s=0}p(T_{s,n})\right\}P_n\right]\\ &= \lim_{n\to\infty}\int_0^{2\pi}\frac{d^2}{dt^2}\Big(p(e^{it})\Big)\tilde{\eta}_n(t)dt, \qquad (3.57)\end{aligned}$$

where $A_n = P_nAP_n$, $T_{0,n} = P_nT_0P_n$, $T_n = e^{iA_n}T_{0,n}$, $T_{s,n} = e^{isA_n}T_{0,n}$, and

$$\tilde{\eta}_n(t) = \int_0^1 \operatorname{Tr}\left[A_n\left\{\mathcal{F}_{0,n}(t)-\mathcal{F}_{s,n}(t)\right\}\right]ds,\ t\in[0,2\pi], \qquad (3.58)$$

where $\mathcal{F}_{0,n}(\cdot)$, $\mathcal{F}_{s,n}(\cdot)$ are corresponding semi-spectral measures of the contractions $T_{0,n}$ and $T_{s,n}$ respectively. Moreover, from (3.14) it follows that

$$\big\|[\tilde{\eta}_n]\big\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} \le \frac{1}{2}\,\|A_n\|_2^2. \qquad (3.59)$$

Next we show that the sequence $\{\tilde{\eta}_n\}$ converges in some suitable sense. Indeed, using the similar setup as in the proof of the Theorem 3.5.1, we have for $f\in\mathcal{P}(\mathbb{T})$ and $g(e^{it}) = \int_0^t f(e^{is})ie^{is}ds$, $t\in[0,2\pi]$ that

$$\begin{aligned}&\int_{\mathbb{T}} f(z)\{\tilde{\xi}_n(z)-\tilde{\xi}_m(z)\}dz = \int_0^{2\pi} f(e^{it})\{\tilde{\eta}_n(e^{it})-\tilde{\eta}_m(e^{it})\}\ ie^{it}dt\\ &= \int_0^{2\pi}\frac{d}{dt}\{g(e^{it})\}\left[\int_0^1\operatorname{Tr}\left[A_n\left\{\mathcal{F}_{0,n}(t)-\mathcal{F}_{s,n}(t)\right\}-A_m\left\{\mathcal{F}_{0,m}(t)-\mathcal{F}_{s,m}(t)\right\}\right]ds\right]dt, \qquad (3.60)\end{aligned}$$

where we set $\tilde{\xi}_n(z) = \tilde{\eta}_n(Arg(z))$, $z\in\mathbb{T}$. Next by using Fubini's theorem to interchange the orders of integration and integrating by-parts, the above expression (3.60) becomes

$$\begin{aligned}&\int_{\mathbb{T}} f(z)\{\tilde{\xi}_n(z)-\tilde{\xi}_m(z)\}dz\\ &= \int_0^1 ds\ \operatorname{Tr}\Bigg[A_n\Bigg\{\Big\{g(T_{s,n})-g(T_s)\Big\}-\Big\{g(T_{0,n})-g(T_0)\Big\}\Bigg\}\\ &\qquad - A_m\Bigg\{\Big\{g(T_{s,m})-g(T_s)\Big\}-\Big\{g(T_{0,m})-g(T_0)\Big\}\Bigg\}+(A_n-A_m)\Big\{g(T_s)-g(T_0)\Big\}\Bigg],\end{aligned}$$

which by using Theorem 3.2.2 yields

$$\begin{aligned}\left|\int_{\mathbb{T}} f(z)\{\tilde{\xi}_n(z)-\tilde{\xi}_m(z)\}dz\right| \le\ & \int_0^1\Big[\|A\|_2\|f\|_\infty\Big[\,\|T_{s,n}P_n-P_nT_s\|_2+\|T_{0,n}P_n-P_nT_0\|_2\\ &+\|T_{s,m}P_m-P_mT_s\|_2+\|T_{0,m}P_m-P_mT_0\|_2\Big]+\|f\|_\infty\|(A_n-A_m)\|_2\,\|T_s-T_0\|_2\Big]\ ds,\end{aligned}$$

and hence by applying Lemma 3.2.1 we have

$$\left\|[\tilde{\xi}_n] - [\tilde{\xi}_m]\right\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} = \left\|[\tilde{\xi}_n - \tilde{\xi}_m]\right\|_{L^1(\mathbb{T})/H^1(\mathbb{T})} = \sup_{f\in\mathcal{P}(\mathbb{T});\ \|f\|_\infty\leq 1} \left|\int_{\mathbb{T}} f(z)\{\tilde{\xi}_n(z) - \tilde{\xi}_m(z)\}dz\right|$$

$$\leq \int_0^1 \Big[\|A\|_2 \left[\|T_{s,n}P_n - P_nT_s\|_2 + \left\|P_nT_0P_n^\perp\right\|_2 + \|T_{s,m}P_m - P_mT_s\|_2 + \left\|P_mT_0P_m^\perp\right\|_2\right] + \|(A_n - A_m)\|_2 \left\|T_s - T_0\right\|_2\Big] \, ds. \tag{3.61}$$

Finally, using the estimates listed in Lemma 3.4.3 we conclude that the right hand side of (3.61) converges to zero as $m, n \longrightarrow \infty$. Therefore $\left\{[\tilde{\xi}_n]\right\}$ is a Cauchy sequence in $L^1(\mathbb{T})/H^1(\mathbb{T})$ and hence there exists a $\tilde{\xi} \in L^1(\mathbb{T})$ such that $\left\{[\tilde{\xi}_n]\right\}$ converges to $[\tilde{\xi}]$ in $L^1(\mathbb{T})/H^1(\mathbb{T})$-norm which by using (3.57) yields

$$\operatorname{Tr}\left\{p(T) - p(T_0) - \frac{d}{ds}\bigg|_{s=0} p(T_s)\right\} = \int_0^{2\pi} \frac{d^2}{dt^2}\left\{p(e^{it})\right\}\tilde{\xi}(e^{it})dt = \int_0^{2\pi} \frac{d^2}{dt^2}\left\{p(e^{it})\right\}\tilde{\eta}(t)dt,$$

where $\tilde{\eta}(t) = \tilde{\xi}(e^{it})$ $t \in [0, 2\pi]$. Moreover, using the estimate (3.59) and applying the definition of the $L^1(\mathbb{T})/H^1(\mathbb{T})$- norm we conclude the estimate (3.56). This completes the proof. □

Remark 3.9.2. *By repeating the similar argument as given in the proof of Theorem 2.4.3, the above Theorem 3.9.1 can also be extended to the class* $\mathcal{F}_2^+(\mathbb{T})$.

CHAPTER 4

Higher-order spectral shift for pairs of contractions via multiplicative path

4.1 Introduction

In the previous chapters, that is, in Chapter 2, and Chapter 3, we briefly discussed first and second order trace formulae in various cases. In 2013, Potapov, Skripka, and Sukochev affirmatively resolved Koplienko's conjecture in [53] using an important and advanced tool in perturbation theory, namely Multiple Operator Integrals (MOI), and proved the following:

$$\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right) = \int_{\mathbb{R}} f^{(n)}(\lambda)\eta_n(\lambda)d\lambda, \text{ where } \mathcal{R}_{H_0,f,n}(V) := f(H_0+V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\bigg|_{s=0} f(H_s), \tag{4.1}$$

for every sufficiently smooth function f, $H_s = H_0 + sV$, $s \in \mathbb{R}$, and $f^{(n)}$ denotes the n-th order derivative of f, where H and H_0 are two self-adjoint operators in a separable Hilbert space $\mathcal{H}$ such that $H - H_0 = V \in \mathcal{B}_n(\mathcal{H})$ (n-th Schatten-von Neumann ideal), and the spectral shift function η_n (of order $n \in \mathbb{N}$) is integrable on $\mathbb{R}$ and depends only on H, H_0, and n. For more on the Koplienko trace formula, we refer to [22, 23, 26, 64] and the references cited therein.

In 2014, for general $n(\geq 3) \in \mathbb{N}$, Potapov, Skripka and Sukochev obtained the formula (4.1) for any pair of contractions U_0 and $U_0 + V$ with the perturbation $V \in \mathcal{B}_n(\mathcal{H})$ via linear path in [54, Theorem 1.3]. In other words, they proved the following result:

Theorem 4.1.1. *(See [54, Theorem 1.3]) Let $n \in \mathbb{N}$, $n \geq 3$. Let U_1 and U_0 be two contractions on a separable Hilbert space $\mathcal{H}$, $V := U_1 - U_0 \in \mathcal{B}_n(\mathcal{H})$ and denote $U_s = U_0 + sV$, $s \in [0,1]$. Then for any complex polynomial f, $\mathcal{R}_{U_0,f,n}(V) \in \mathcal{B}_1(\mathcal{H})$ and there exists $L^1(\mathbb{T})$-function $\eta_n = \eta_{n,U_0,V}$ such that*

$$\operatorname{Tr}\left(\mathcal{R}_{U_0,f,n}(V)\right) = \int_{\mathbb{T}} f^{(n)}(z)\eta_n(z)dz. \tag{4.2}$$

Furthermore, for every given $\epsilon > 0$, the function η_n satisfying (4.2) can be chosen so that $\|\eta_n\|_1 \leq (1+\epsilon)c_n\|V\|_n^n$, where c_n is some constant.

Going further, in 2016, for general $n(\geq 2) \in \mathbb{N}$, Potapov, Skripka and Sukochev established the formula (4.1) for the couple of unitaries U_0 and $U_1 = e^{iA}U_0$ with the perturbation $A = A^* \in \mathcal{B}_n(\mathcal{H})$ via multiplicative path in [55, Theorem 4.1] corresponding to the class $\mathcal{F}_{nn}^{+}(\mathbb{T})$. More precisely, Skripka obtained the following result, and it will be useful to achieve our main results in later sections:

Theorem 4.1.2. *(See [55, Theorem 4.1]) Let $n \in \mathbb{N}$, $n \geq 2$. Let U_0 be a unitary operator, $A = A^* \in \mathcal{B}_n(\mathcal{H})$ and denote $U_s = e^{isA}U_0$, $s \in [0,1]$. Then, for any $f \in \mathcal{F}_{nn}^{+}(\mathbb{T})$, $\mathcal{R}_{U_0,f,n}(V) \in \mathcal{B}_1(\mathcal{H})$ and there exists a constant c_n and a function $\eta_n = \eta_{n,U_0,A} \in L^1([0,2\pi])$ satisfying $\|\eta_n\|_1 \leq c_n\|A\|_n^n$ such that*

$$\operatorname{Tr}\left\{f(U_1) - f(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k}\Big|_{s=0} f(U_s)\right\} = \int_0^{2\pi} f^{(n)}(e^{it})\eta_n(t)dt.$$

Later, in 2017, Skripka extended the associated class of scalar functions in the above Theorem 4.1.2 from $\mathcal{F}_{nn}^{+}(\mathbb{T})$ to $\mathcal{F}_n(\mathbb{T})$ (see [66, Theorem 4.4]).

In this direction of studies, Marcantognini and Morán obtained the Koplienko-Neidhardt trace formula (second order trace formula) for pairs of contraction operators and pairs of maximal dissipative operators via multiplicative path in [40]. The present chapter aims to prove a higher-order version of the Koplienko-Neidhardt trace formula for pairs of contractions and pairs of maximal dissipative operators via multiplicative path by adapting the method developed for the second order trace formula in [40]. The novelty of our results is that the extension is natural in comparison with the known higher-order trace formulas for unitary and self-adjoint operators. Moreover, the importance of our work lies in the fact that our results provide some new addition to the theory of spectral shift functions. One of the major ingredients to prove our main result is the higher-order trace formulas for unitary operators, namely Theorem 4.1.2. We have adapted the method applied in [40] and modified it appropriately to obtain our main results in this chapter. The major tools required to achieve our results are the Schäffer matrix unitary dilation and the Cayley transformation. In other words, the transference of the trace formulas from unitary to contractive operators is made by means of the dilation theory, and the transference from the contractive to dissipative operators is made with the help of the Cayley transform as done in [40]. More precisely, the following are the major contributions of this chapter:

(A) First, we prove a higher-order version of [40, Theorem 2.1]. In other words, we consider a pair (T, V), where V is a unitary operator and T is a contraction on $\mathcal{H}$. Then we prove a higher-order version of the Koplienko-Neidhardt trace formula via multiplicative path corresponding to the pair (T, V) under some additional hypotheses (see Theorem 4.3.2) by using dilation theory and applying Theorem 4.1.2.

(B) Next, we obtain a higher-order version of [40, Theorem 2.3]. More precisely, we prove a higher-order version of the Koplienko-Neidhardt trace formula via multiplicative path for pairs of contractions (T_0, T_1) (see Theorem 4.4.1) by using our Theorem 4.3.2.

(C) At the end, we prove a higher-order version of [40, Theorem 2.3]. In other words, as an application of our Theorem 4.4.1 for pairs of contractions, we obtain a higher-order analogue of the Koplienko-Neidhardt trace formula via multiplicative path for pairs of maximal dissipative operators (see Theorem 4.5.2).

The major difficulties we face in extending the results of [40] to higher-order are as follows:

- Obtain a precise expression of the k-order derivatives $\dfrac{d^k}{ds^k}\Big|_{s=0}\big\{(V_s)^n\big\}$, and $\dfrac{d^k}{ds^k}\Big|_{s=0}\big\{(T_s)^n\big\}$, which we are able to overcome due to [69, Theorem 5.3.4](see (4.17), (4.18)).

- Secondly, to show $P_{\mathcal{H}}X_r\Big|_{\mathcal{H}} = Y_r$ and $P_{\mathscr{F}\ominus\mathcal{H}}X_r\Big|_{\mathscr{F}\ominus\mathcal{H}} = P_{\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})}X_rP_{\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})}\Big|_{\mathscr{F}\ominus\mathcal{H}}$ for $r \geq 2$, which we are able to complete by rigorously analyzing the block matrix representations of the corresponding operators and shifting accordingly the projections from left to right (see (4.9), (5.40), (4.26), (4.27), and (4.28)).

The rest of the chapter is organized as follows: Section 4.2 deals with some essential preliminaries, which will be useful in later sections. In Section 4.3, we prove the higher-order analogue of the Koplienko-Neidhardt trace formula corresponding to the pair (T, V) via multiplicative path, where V is a unitary operator and T is a contraction on $\mathcal{H}$. Section 4.4 is devoted to obtaining a higher-order version of the Koplienko-Neidhardt trace formula for pairs of contractions via multiplicative path. Consequently, in Section 4.5, we prove the trace formula for pairs of maximal dissipative operators.

4.2 Preliminaries

Notations: Given a closed subspace $\mathcal{M}$ of $\mathcal{H}$, $P_{\mathcal{M}}$ denotes the orthogonal projection of $\mathcal{H}$ onto $\mathcal{M}$.

Recall that $\mathcal{H}$-valued Hardy space over the unit disc $\mathbb{D}$ in $\mathbb{C}$ is denoted by $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ and defined by

$$\mathbf{H}^2_{\mathcal{H}}(\mathbb{D}) := \Big\{ f(z) = \sum_{k=0}^{\infty} a_k z^k : \; \|f\|^2_{\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})} := \sum_{k=0}^{\infty} \|a_k\|^2_{\mathcal{H}} < \infty, \; z \in \mathbb{D}, \; a_k \in \mathcal{H} \Big\}. \tag{4.3}$$

Recall that the shift operator on the Hardy space $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ is denoted by $S_{\mathcal{H}}$ and is defined by $(S_{\mathcal{H}} f)(z) := z f(z), \; f \in \mathbf{H}^2_{\mathcal{H}}(\mathbb{D}), \; z \in \mathbb{D}$. It is easy to check that $S_{\mathcal{H}}$ is an isometry on $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ and $S_{\mathcal{H}} S_{\mathcal{H}}^* = I - P_{\mathcal{H}}$, where $P_{\mathcal{H}}$ is the orthogonal projection of $\mathbf{H}^2_{\mathcal{H}}(\mathbb{D})$ onto $\mathcal{H}$ (that is, by identifying $\mathcal{H}$ as $\mathcal{H}$-valued constant functions). For more on vector valued Hardy space we refer to [44, 45].

Let $T \in \mathcal{B}(\mathcal{H})$ be a contraction, that is $\|T\| \leq 1$. Then the defect operator of T is denoted by D_T and defined by $D_T := (1 - T^*T)^{1/2}$. Moreover, $\mathcal{D}_T := \overline{\operatorname{Ran}(D_T)}$ is known as the corresponding defect space of T. Recall that the minimal unitary dilation (see Chapter 1 Section 1.6) of a contraction T is a unitary operator $U_T : \mathscr{F} = \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \to \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ such that $T^n = P_{\mathcal{H}} U_T^n|_{\mathcal{H}}$ and $T^{*^n} = P_{\mathcal{H}} U_T^{-n}|_{\mathcal{H}}$ for $n \in \mathbb{N}$, and $\mathscr{F}$ is the smallest Hilbert space containing the subspaces $U_T^n \mathcal{H}$ for all $n \in \mathbb{Z}$. Furthermore, the block matrix (Schäffer matrix) representation of U_T is as follows:

$$U_T = \begin{bmatrix} S^*_{\mathcal{D}_{T^*}} & 0 & 0 \\ D_{T^*} P_{\mathcal{D}_{T^*}} & T & 0 \\ -T^* P_{\mathcal{D}_{T^*}} & D_T & S_{\mathcal{D}_T} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \longrightarrow \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}, \tag{4.4}$$

where $S_{\mathcal{D}_T}$ and $S_{\mathcal{D}_{T^*}}$ are the shift operator on $\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ and $\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})$ respectively and $P_{\mathcal{D}_{T^*}}$ is the orthogonal projection from $\mathscr{F}$ onto $\mathcal{D}_{T^*} \oplus \mathbf{0} \oplus \mathbf{0} \equiv \mathcal{D}_{T^*}$. Given a pair of contractions (T_0, T) on $\mathcal{H}$, we denote by $U_{T_0,T}$ the extension of T_0 to the minimal dilation space $\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ of T and the block matrix representation of $U_{T_0,T}$ is given by

$$U_{T_0,T} := \begin{bmatrix} S^*_{\mathcal{D}_{T^*}} & 0 & 0 \\ 0 & T_0 & 0 \\ -V_T^* P_{\mathcal{D}_{T^*}} & 0 & S_{\mathcal{D}_T} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \longrightarrow \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}. \tag{4.5}$$

For more on dilation theory we refer to [70].

4.3 Higher-order Trace formula for pair of contractive operators with one of them is unitary

In this section, we prove the higher-order version of the Koplienko-Neidhardt trace formula via multiplicative path for a pair (T, V), where T is a contraction and V is a unitary operator on $\mathcal{H}$ such that $T - V \in \mathcal{B}_n(\mathcal{H})$. To proceed further, we need the following auxiliary lemma towards obtaining our main result in this section. Note that Lemma 4.3.1 below is available in [69, Theorem 5.3.4] in the case when U is a unitary operator and the expression of the k-th order Gâteaux derivative of $f(U_t)$ is given in terms of multiple operator integral, where f belongs to the Besov space. On the other hand, in our case, U is a contraction, and f is a polynomial. Nevertheless, by following the same lines of proof of [69, Theorem 5.3.4], we obtain the following Lemma 4.3.1.

Lemma 4.3.1. *Let $p(z) = z^n$, $z \in \mathbb{T}$ and $n \in \mathbb{N}$, let $A \in \mathcal{B}(\mathcal{H})$ be a self-adjoint operator and let $U \in \mathcal{B}(\mathcal{H})$. Set $U_t = e^{itA}U$, $t \in \mathbb{R}$. Then for all $1 \le k \le n-1$, we have*

$$\frac{d^k}{dt^k}\Big|_{t=s}\{U_t^n\} = \sum_{r=1}^{k} \sum_{\substack{l_1+l_2+\cdots+l_r=k \\ l_1,l_2,\ldots,l_r \ge 1}} \frac{k!}{l_1!\cdots l_r!}\left[\sum_{\substack{\alpha_0+\alpha_1+\cdots+\alpha_r=n-r \\ \alpha_0,\alpha_1,\ldots,\alpha_r \ge 0}} U_s^{\alpha_0} W_s^{l_1} U_s^{\alpha_1}\cdots W_s^{l_r} U_s^{\alpha_r}\right], \tag{4.6}$$

where $W_s^l = \left((iA)^l e^{isA} U\right)$, $l \in \mathbb{N}$.

Proof. We prove the lemma by applying mathematical induction on k. For $k = 1$, using the definition of Gâteaux derivative we get

$$\frac{d}{dt}\Big|_{t=s}\{U_t^n\} = \lim_{h\to 0}\frac{U_{s+h}^n - U_s^n}{h} = \lim_{h\to 0}\sum_{j=0}^{n-1} U_{s+h}^{n-j-1}\left(\frac{U_{s+h}-U_s}{h}\right)U_s^j$$
$$= \sum_{j=0}^{n-1} U_s^{n-j-1}\left(iAe^{isA}U\right)U_s^j = \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_0,\alpha_1\geq 0}} U_s^{\alpha_0}W_s^1U_s^{\alpha_1}.$$

Similarly for $k = 2$, again by using the definition of Gâteaux derivative we have

$$\frac{d^2}{dt^2}\Big|_{t=s}\{U_t^n\} = \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_0\geq 1\ \&\ \alpha_1\geq 0}}\ \sum_{\substack{\beta_0+\beta_1=\alpha_0-1\\ \beta_0,\beta_1\geq 0}} U_s^{\beta_0}W_s^1U_s^{\beta_1}W_s^1U_s^{\alpha_1}$$
$$+ \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_1\geq 1\ \&\ \alpha_0\geq 0}}\ \sum_{\substack{\beta_0+\beta_1=\alpha_1-1\\ \beta_0,\beta_1\geq 0}} U_s^{\alpha_0}W_s^1U_s^{\beta_0}W_s^1U_s^{\beta_1} + \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_0,\alpha_1\geq 0}} U_s^{\alpha_0}W_s^2U_s^{\alpha_1}$$
$$=2!\sum_{\substack{\alpha_0+\alpha_1+\alpha_2=n-2\\ \alpha_0,\alpha_1,\alpha_2\geq 0}} U_s^{\alpha_0}W_s^1U_s^{\alpha_1}W_s^1U_s^{\alpha_2} + \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_0,\alpha_1\geq 0}} U_s^{\alpha_0}W_s^2U_s^{\alpha_1}$$
$$=\sum_{r=1}^{2}\ \sum_{\substack{l_1+l_2+\cdots+l_r=2\\ l_1,l_2,\ldots,l_r\geq 1}} \frac{2!}{l_1!\cdots l_r!}\left[\sum_{\substack{\alpha_0+\alpha_1+\cdots+\alpha_r=n-r\\ \alpha_0,\alpha_1,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0}W_s^{l_1}U_s^{\alpha_1}\cdots W_s^{l_r}U_s^{\alpha_r}\right].$$

Therefore the result is true for $k = 1, 2$. Now we assume that the result holds for $k = q < n-1$, that is the equation (4.6) is true for $k = q$. Next we show that the equation (4.6) also holds for $k = q+1$. Now by applying Leibnitz rule for Gâteaux derivative and using induction hypothesis we get

$$\frac{d^{q+1}}{dt^{q+1}}\Big|_{t=s}\{U_t^n\}$$
$$=\sum_{r=1}^{q}\ \sum_{\substack{l_1+\cdots+l_r=q\\ l_1,l_2,\ldots,l_r\geq 1}} \frac{q!}{l_1!\cdots l_r!}\frac{d}{dt}\Big|_{t=s}\left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\alpha_1,\ldots,\alpha_r\geq 0}} U_t^{\alpha_0}W_t^{l_1}U_t^{\alpha_1}\cdots W_t^{l_r}U_t^{\alpha_r}\right]$$
$$=\sum_{r=1}^{q}\ \sum_{\substack{l_1+\cdots+l_r=q\\ l_1,\ldots,l_r\geq 1}} \frac{q!}{l_1!\cdots l_r!}$$
$$\times\sum_{k=1}^{r}\left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0}W_s^{l_1}U_s^{\alpha_1}\cdots W_s^{l_{k-1}}U_s^{\alpha_{k-1}}W_s^{l_k+1}U_s^{\alpha_k}W_s^{l_{k+1}}\cdots W_s^{l_r}U_s^{\alpha_r}\right]$$
$$+\sum_{r=1}^{q}\ \sum_{\substack{l_1+\cdots+l_r=q\\ l_1,\ldots,l_r\geq 1}} \frac{q!}{l_1!\cdots l_r!}$$

$$\times \sum_{k=1}^{r+1} \left[\sum_{\substack{\alpha_0+\cdots+\alpha_{r+1}=n-(r+1)\\ \alpha_0,\ldots,\alpha_{r+1}\geq 0}} U_s^{\alpha_0} W_s^{l_1} U_s^{\alpha_1} \cdots W_s^{l_{k-1}} U_s^{\alpha_{k-1}} W_s^{1} U_s^{\alpha_k} W_s^{l_k} U_s^{\alpha_{k+1}} \cdots W_s^{l_r} U_s^{\alpha_{r+1}} \right]$$

$$= K_1 + K_2 \text{ (say)}.$$

Now if we substitute $j_a = l_a, 1 \leq a \neq k \leq r$ and $j_k = l_k + 1$ in K_1, we obtain

$$K_1 = \sum_{r=1}^{q} \sum_{k=1}^{r} \sum_{\substack{j_1+\cdots+j_r=q+1\\ j_a\geq 1, a\neq k, j_k\geq 2}} \frac{q!}{j_1! \cdots j_{k-1}!(j_k-1)! \cdots j_r!}$$
$$\times \left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0} W_s^{j_1} U_s^{\alpha_1} \cdots W_s^{j_{k-1}} U_s^{\alpha_{k-1}} W_s^{j_k} U_s^{\alpha_k} W_s^{j_{k+1}} \cdots W_s^{j_r} U_s^{\alpha_r} \right].$$

On the other hand, by relabeling the summands of K_2 via $r \mapsto r-1$ and performing the substitution $j_a = l_a, 1 \leq a \leq k-1, j_k = 1$, and $j_a = l_{a-1}, k+1 \leq a \leq r$, we obtain

$$K_2 = \sum_{r=2}^{q+1} \sum_{\substack{l_1+\cdots+l_{r-1}=q\\ l_1,\ldots,l_{r-1}\geq 1}} \frac{q!}{l_1! \cdots l_{r-1}!}$$
$$\times \sum_{k=1}^{r} \left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0} W_s^{l_1} U_s^{\alpha_1} \cdots W_s^{l_{k-1}} U_s^{\alpha_{k-1}} W_s^{1} U_s^{\alpha_k} W_s^{l_k} U_s^{\alpha_{k+1}} \cdots W_s^{l_{r-1}} U_s^{\alpha_r} \right]$$
$$= \sum_{r=2}^{q+1} \sum_{k=1}^{r} \sum_{\substack{j_1+\cdots+j_r=q+1\\ j_a\geq 1, j_k=1}} \frac{q!}{j_1! \cdots j_{k-1}! \cdot j_{k+1}! \ldots j_r!} \left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0} W_s^{j_1} \cdots W_s^{j_r} U_s^{\alpha_r} \right].$$

Thus,

$$K_1 + K_2 = \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_0,\alpha_1\geq 0}} U_s^{\alpha_0} W_s^{q+1} U_s^{\alpha_1}$$
$$+ \sum_{r=2}^{q} \sum_{k=1}^{r} \left[\sum_{\substack{j_1+\cdots+j_r=q+1\\ j_a\geq 1, a\neq k, j_k\geq 2}} + \sum_{\substack{j_1+\cdots+j_r=q+1\\ j_a\geq 1, j_k=1}} \right] \frac{q!}{j_1! \cdots j_{k-1}!(j_k-1)! \cdots j_r!}$$
$$\times \left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0} W_s^{j_1} \cdots W_s^{j_r} U_s^{\alpha_r} \right]$$
$$+ \sum_{k=1}^{q+1} \sum_{\substack{j_1+\cdots+j_{q+1}=q+1\\ j_a\geq 1, j_k=1}} \frac{q!}{j_1! \cdots j_{k-1}!(j_k-1)! \cdots j_{q+1}!}$$
$$\times \left[\sum_{\substack{\alpha_0+\cdots+\alpha_{q+1}=n-(q+1)\\ \alpha_0,\ldots,\alpha_{q+1}\geq 0}} U_s^{\alpha_0} W_s^{j_1} \cdots W_s^{j_{q+1}} U_s^{\alpha_{q+1}} \right]$$

$$= \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_0,\alpha_1\geq 0}} U_s^{\alpha_0} W_s^{q+1} U_s^{\alpha_1}$$
$$+ \sum_{r=2}^{q} \sum_{k=1}^{r} \sum_{\substack{j_1+\cdots+j_r=q+1\\ j_1\ldots j_r\geq 1}} \frac{q!}{j_1!\cdots j_{k-1}!(j_k-1)!j_{k+1}\cdots j_r!}$$
$$\times \left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0} W_s^{j_1}\cdots W_s^{j_r} U_s^{\alpha_r}\right]$$
$$+ (q+1)! \sum_{\substack{\alpha_0+\cdots+\alpha_{q+1}=n-(q+1)\\ \alpha_0,\ldots,\alpha_{q+1}\geq 0}} U_s^{\alpha_0} W_s^{1}\cdots W_s^{1} U_s^{\alpha_{q+1}}.$$

Since

$$\sum_{k=1}^{r} \frac{q!}{j_1!\cdots j_{k-1}!(j_k-1)!j_{k+1}\cdots j_r!} = q!\,\frac{(j_1+\cdots+j_r)}{j_1!\cdots j_r!} = \frac{(q+1)!}{j_1!\cdots j_r!},$$

it follows that

$$K_1+K_2 = \sum_{\substack{\alpha_0+\alpha_1=n-1\\ \alpha_0,\alpha_1\geq 0}} U_s^{\alpha_0} W_s^{q+1} C_s^{\alpha_1} + \sum_{r=2}^{q} \sum_{\substack{j_1+\cdots+j_r=q+1\\ j_1\ldots j_r\geq 1}} \frac{(q+1)!}{j_1!\cdots j_r!}$$
$$\times \left[\sum_{\substack{\alpha_0+\cdots+\alpha_r=n-r\\ \alpha_0,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0} W_s^{j_1}\cdots W_s^{j_r} U_s^{\alpha_r}\right]$$
$$+ (q+1)! \sum_{\substack{\alpha_0+\cdots+\alpha_{q+1}=n-(q+1)\\ \alpha_0,\ldots,\alpha_{m+1}\geq 0}} U_s^{\alpha_0} W_s^{1}\cdots W_s^{1} U_s^{\alpha_{q+1}}$$
$$= \sum_{r=1}^{q+1} \sum_{\substack{j_1+\cdots+j_r=q+1\\ j_1,\ldots,l_r\geq 1}} \frac{(q+1)!}{j_1!\cdots j_r!} \left[\sum_{\substack{\alpha_0+\alpha_1+\cdots+\alpha_r=n-r\\ \alpha_0,\alpha_1,\ldots,\alpha_r\geq 0}} U_s^{\alpha_0} W_s^{j_1} U_s^{\alpha_1}\cdots W_s^{j_r} U_s^{\alpha_r}\right].$$

Therefore the identity (4.6) is true for $k = q+1$ and hence by principle of mathematical induction (4.6) is true for each $q \in \mathbb{N}$. This completes the proof.

□

Now we are in a position to state and prove our main result in this section.

Theorem 4.3.2. *Let $n \in \mathbb{N}$, $n \geq 2$. Let T and V be two contractions in $\mathcal{H}$ such that*

(i) $V^*V = VV^* = I$, and $\dim(\ker T) = \dim(\ker T^*)$,

(ii) $T - V \in \mathcal{B}_n(\mathcal{H})$, and $(I - T^*T)^{1/2} \in \mathcal{B}_n(\mathcal{H})$.

Let $T = V_T|T|$ be the polar decomposition of T, where V_T is a partial isometry on $\mathcal{H}$ and $|T| = (T^*T)^{1/2}$. Set $\mathcal{L} := \begin{bmatrix} TV^* & -D_{T^*}V_T\big|_{\mathcal{D}_T} \\ D_TV^* & T^*V_T\big|_{\mathcal{D}_T} \end{bmatrix} : \begin{bmatrix} \mathcal{H} \\ \\ \mathcal{D}_T \end{bmatrix} \longrightarrow \begin{bmatrix} \mathcal{H} \\ \\ \mathcal{D}_T \end{bmatrix}$. Then $\mathcal{L}$ is a unitary operator on $\mathcal{H} \oplus \mathcal{D}_T$ and, hence there exists a unique self-adjoint operator $L \in \mathcal{B}_n(\mathcal{H} \oplus \mathcal{D}_T)$ with $\sigma(L) \subseteq (-\pi, \pi]$ such that $\mathcal{L} = e^{iL}$. Furthermore, if we denote $V_s := P_{\mathcal{H}} e^{isL} V, s \in [0,1]$, then for $\phi \in \mathcal{F}^+_{nn}(\mathbb{T})$ (see (1.8)),

$$\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(V_s)\right\} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists an $L^1([0, 2\pi])$-function ξ_n depend only on n, T and V such that

$$\operatorname{Tr}\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(V_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it}) \xi_n(t) dt. \tag{4.7}$$

To prove the above theorem we need the following lemma.

Lemma 4.3.3. *Assume notations and hypotheses of the above Theorem 4.3.2. Let $U_1 := U_T$ and $U_0 = U_{T_0,T}$. Let*

$$\begin{aligned}
\mathscr{F} &:= \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}), \quad X_0 := U_1^n - U_0^n, \quad Y_0 := T^n - V^n, \\
X_r &:= U_0^{\alpha_0}((iA)^{l_1} U_0)\, U_0^{\alpha_1} \cdots ((iA)^{l_r} U_0) U_0^{\alpha_r}, \text{ and} \\
Y_r &:= V^{\alpha_0} P_{\mathcal{H}}((iL)^{l_1} V) V^{\alpha_1} \cdots V^{\alpha_{r-1}} P_{\mathcal{H}}((iL)^{l_r} V) V^{\alpha_r},
\end{aligned}$$

where A, L are given in (4.12), $\alpha_j \geq 0$ for $0 \leq j \leq r$, and $l_{j'} \geq 1$ for $1 \leq j' \leq r$, and $r \geq 1$. Then for every integer $r \geq 0$,

(i) $P_{\mathcal{H}} X_r\big|_{\mathcal{H}} = Y_r$.

(ii) $P_{\mathscr{F} \ominus \mathcal{H}} X_r\big|_{\mathscr{F} \ominus \mathcal{H}} = P_{\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})} X_r P_{\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})}\big|_{\mathscr{F} \ominus \mathcal{H}}$.

Proof. For $r = 0$, it is clear from the structures of U_1 and U_0 that

$$P_{\mathcal{H}} X_r\big|_{\mathcal{H}} = Y_r. \tag{4.8}$$

For $r \geq 1$, by analyzing the block matrix representations (4.4), (4.5) and (4.12) of U_1, U_0 and A respectively, we conclude

$$P_{\mathcal{H}} X_r\big|_{\mathcal{H}} = P_{\mathcal{H}} U_0^{\alpha_0}((iA)^{l_1} U_0) U_0^{\alpha_1} \cdots ((iA)^{l_r} U_0) U_0^{\alpha_r}\big|_{\mathcal{H}}$$

$$
\begin{aligned}
&= P_{\mathcal{H}} U_0^{\alpha_0} P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_1} P_{\mathcal{H}\oplus\mathcal{D}_T} U_0) U_0^{\alpha_1} P_{\mathcal{H}\oplus\mathcal{D}_T} \cdots U_0^{\alpha_{r-1}} P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_r} P_{\mathcal{H}\oplus\mathcal{D}_T} U_0) U_0^{\alpha_r}\Big|_{\mathcal{H}} \\
&= V^{\alpha_0} P_{\mathcal{H}}((iL)^{l_1} V) V^{\alpha_1} \cdots V^{\alpha_{r-1}} P_{\mathcal{H}}((iL)^{l_r} V) V^{\alpha_r} = Y_r. \qquad (4.9)
\end{aligned}
$$

On the other hand, for $r = 0, 1$, it was obtained in the proof of [40, Theorem 2.1] that

$$
P_{\mathscr{F}\ominus\mathcal{H}} X_r\Big|_{\mathscr{F}\ominus\mathcal{H}} = P_{\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})} X_r P_{\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})}\Big|_{\mathscr{F}\ominus\mathcal{H}}.
$$

For $r \geq 2$, by analyzing the structures of U_1, U_0, and A as in (4.4), (4.5), and (4.12) respectively we get

$$
\begin{aligned}
P_{\mathscr{F}\ominus\mathcal{H}} X_r\Big|_{\mathscr{F}\ominus\mathcal{H}} &= P_{\mathscr{F}\ominus\mathcal{H}} U_0^{\alpha_0}((iA)^{l_1} U_0) U_0^{\alpha_1} \cdots ((iA)^{l_r} U_0) U_0^{\alpha_r}\Big|_{\mathscr{F}\ominus\mathcal{H}} \\
&= P_{\mathscr{F}\ominus\mathcal{H}} U_0^{\alpha_0} P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_1} P_{\mathcal{H}\oplus\mathcal{D}_T} U_0) U_0^{\alpha_1} \cdots P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_r} P_{\mathcal{H}\oplus\mathcal{D}_T} U_0) U_0^{\alpha_r}\Big|_{\mathscr{F}\ominus\mathcal{H}} \\
&= P_{\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})} U_0^{\alpha_0} P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_1} P_{\mathcal{H}\oplus\mathcal{D}_T} U_0) U_0^{\alpha_1} \\
&\qquad \times \cdots \times P_{\mathcal{H}\oplus\mathcal{D}_T}((iA)^{l_r} P_{\mathcal{H}\oplus\mathcal{D}_T} U_0) U_0^{\alpha_r} P_{\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D})}\Big|_{\mathscr{F}\ominus\mathcal{H}}. \qquad (4.10)
\end{aligned}
$$

□

Proof of Theorem 4.3.2. Let $U_1 := U_T$ be the corresponding minimal unitary dilation of T on $\mathscr{F} = \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$. Given that $T = V_T|T|$ is the polar decomposition of T, where $|T| = (T^*T)^{1/2}$ and V_T is an isometry from $\overline{Ran(T^*)}$ onto $\overline{Ran(T)}$. Therefore by using the hypothesis $\dim(\ker T) = \dim(\ker T^*)$, we can extend V_T to a unitary operator on the full space $\mathcal{H}$. Going further, we need the following useful relations obtained in [40]

$$
V_T D_T = D_{T^*} V_T, \ (1 - |T|) = (1 + |T|)^{-1}(1 - T^*T), \ \text{and} \ V_T - T = V_T(1 - |T|). \qquad (4.11)
$$

Let $U_0 := U_{V,T} : \mathscr{F} \to \mathscr{F}$. Now by using the relations listed in (4.11) along with the hypothesis (ii) we conclude $U_1 - U_0 \in \mathcal{B}_n(\mathcal{F})$. Thus, we have a pair (U_1, U_0) of unitary operators on $\mathscr{F}$. By a similar computations as done in the proof of [40, Theorem 2.1], we get a self-adjoint operator $A \in \mathcal{B}_n(\mathscr{F})$ such that $U_1 = e^{iA} U_0$ and the block matrix representation of A with respect to the decomposition $\mathscr{F} = \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus (\mathcal{H} \oplus \mathcal{D}_T) \oplus S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ is the following:

$$
A := \begin{bmatrix} 0 & 0 & 0 \\ 0 & L & 0 \\ 0 & 0 & 0 \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathcal{H} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}. \qquad (4.12)
$$

Therefore the pair (U_1, U_0) satisfies the hypothesis of Theorem 5.2.8 and hence for any $\phi \in \mathcal{F}_{nn}^{+}(\mathbb{T})$,

$$\left\{\phi(U_1) - \phi(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(U_s)\right\} \in \mathcal{B}_1(\mathcal{H}), \tag{4.13}$$

and there exists an $L^1([0, 2\pi])$-function $\eta_n = \eta_{n,U_0,A}$ such that

$$\operatorname{Tr}\left\{\phi(U_1) - \phi(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(U_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it}) \eta_n(t) dt, \tag{4.14}$$

where $U_s = e^{isA} U_0,\ s \in [0, 1]$. Our next aim is to show that for $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\operatorname{Tr}\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(V_s)\right\} = \operatorname{Tr}\left\{\phi(U_1) - \phi(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(U_s)\right\}, \tag{4.15}$$

where

$$V_s := P_{\mathcal{H}} e^{isA} U_0\Big|_{\mathcal{H}} = P_{\mathcal{H}} e^{isL} V,\ \ s \in [0, 1]. \tag{4.16}$$

To this end, it is enough to deal with the monomials, that is functions like $\phi_q(z) = z^q,\ z \in \mathbb{T}$ and $q \in \mathbb{N}$. By using Lemma 4.3.1, we conclude for $1 \leq k \leq n-1$ that

$$\frac{d^k}{ds^k}\Big|_{s=0} \{\phi_q(U_s)\} = \sum_{r=1}^{k} \sum_{\substack{\alpha_0+\cdots+\alpha_r=q-r \\ \alpha_0,\ldots,\alpha_r \geq 0}} \sum_{\substack{l_1+\cdots+l_r=k \\ l_1,\ldots,l_r \geq 1}} \frac{k!}{l_1! \cdots l_r!} U_0^{\alpha_0} ((iA)^{l_1} U_0) U_0^{\alpha_1} \cdots ((iA)^{l_r} U_0) U_0^{\alpha_r}, \tag{4.17}$$

and

$$\frac{d^k}{ds^k}\Big|_{s=0} \{\phi_q(V_s)\} = \sum_{r=1}^{k} \sum_{\substack{\alpha_0+\cdots+\alpha_r=q-r \\ \alpha_0,\ldots,\alpha_r \geq 0}} \sum_{\substack{l_1+\cdots+l_r=k \\ l_1,\ldots,l_r \geq 1}} \frac{k!}{l_1! \cdots l_r!} V^{\alpha_0} P_{\mathcal{H}}((iL)^{l_1} V) V^{\alpha_1} \cdots P_{\mathcal{H}}((iL)^{l_r} V) V^{\alpha_r}. \tag{4.18}$$

Therefore using Lemma 4.3.3 (i), from (4.17) and (4.18) we conclude that

$$\phi_q(T) - \phi_q(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(V_s) = P_{\mathcal{H}} \left(\phi_q(U_1) - \phi_q(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(U_s)\right)\Bigg|_{\mathcal{H}}, \tag{4.19}$$

for all $q \in \mathbb{N}$. Again using Lemma 4.3.3 (ii), we conclude that the operator

$$P_{\mathscr{F} \ominus \mathcal{H}} \left(\phi_q(U_1) - \phi_q(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(U_s)\right)\Bigg|_{\mathscr{F} \ominus \mathcal{H}}$$

maps $\mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus \mathbf{0} \oplus \mathbf{0}$ to $\mathbf{0} \oplus \mathbf{0} \oplus \mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ for $q \in \mathbb{N}$. These observations immediately yield that

$$\operatorname{Tr}\left\{ P_{\mathscr{F}\ominus\mathcal{H}} \left(\phi_q(U_1) - \phi_q(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(U_s) \right) \Big|_{\mathscr{F}\ominus\mathcal{H}} \right\} = 0, \quad \forall q \in \mathbb{N}. \tag{4.20}$$

Therefore combining equations (4.19) and (4.20), we conclude

$$\operatorname{Tr}\left\{ \phi_q(T) - \phi_q(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(V_s) \right\} = \operatorname{Tr}\left\{ \phi_q(U_1) - \phi_q(U_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi_q(U_s) \right\}$$

for all $q \in \mathbb{N}$ and hence (4.15) follows. Finally the conclusion of the theorem follows by combining equations (4.14) and (4.15). This completes the proof. □

4.4 Higher-order Trace formula for pair of contractions

In the previous section, we discuss the trace formula for pairs of contractions (T, V) assuming that V is unitary. In this section, we remove the assumption on V. In other words, we prove the trace formula for pairs of contractions (T_0, T_1) on $\mathcal{H}$. The technique involved here is standard and similar to the idea mentioned in [40] with an appropriate modification, that means first we dilate (T_0, T_1) to a pair of contractions (T, V) with V is a unitary operator on the bigger space $\mathscr{F}$ containing $\mathcal{H}$ as a subspace and then use the existing trace formula for the pair (T, V) obtained in our last section to get the required trace formula in this section. The following is the main result in this section.

Theorem 4.4.1. *Let $n \in \mathbb{N}$, $n \geq 2$. Let T_0 and T_1 be two contractions in $\mathcal{H}$ such that*

(*i*) $\dim(\ker T_0) = \dim(\ker T_0^*)$, *and* $\dim(\ker T_1) = \dim(\ker T_1^*)$,

(*ii*) $T_1 - T_0 \in \mathcal{B}_n(\mathcal{H})$, *and* $(I - T_j^* T_j)^{1/2} \in \mathcal{B}_n(\mathcal{H})$ *for* $j = 0, 1$.

Let $T_j = V_{T_j}|T_j|$ be the polar decomposition of T_j, where V_{T_j} is a partial isometry on $\mathcal{H}$ and $|T_j| = (T_j^* T_j)^{1/2}$ for $j = 0, 1$. Set

$$\mathcal{M} := \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & T_1 T_0^* & T_1 D_{T_0} P_{\mathcal{D}_{T_0}} & -D_{T_1^*} V_{T_1} \\ 0 & -V_{T_0}^* D_{T_0^*} & |T_0| P_{\mathcal{D}_{T_0}} + (I - P_{\mathcal{D}_{T_0}}) & 0 \\ 0 & D_{T_1} T_0^* & D_{T_1} D_{T_0} P_{\mathcal{D}_{T_0}} & T_1^* V_{T_1} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}.$$

Then $\mathcal{M}$ is a unitary operator on $\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \oplus \mathcal{D}_{T_1} = \mathscr{F} \oplus \mathcal{D}_{T_1}$ and hence there exists a unique self-adjoint operator $M \in \mathcal{B}_n(\mathscr{F} \oplus \mathcal{D}_{T_1})$ with $\sigma(M) \subseteq (-\pi, \pi]$ such that $\mathcal{M} = e^{iM}$. Furthermore, if we denote

$$T_s = P_{\mathcal{H}} e^{isM} \begin{bmatrix} 0 \\ T_0 \\ D_{T_0} \\ 0 \end{bmatrix} : \mathcal{H} \to \mathcal{H}, \quad s \in [0,1], \tag{4.21}$$

then for $\phi \in \mathcal{F}^+_{nn}(\mathbb{T})$,

$$\left\{ \phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s) \right\} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists an $L^1([0,2\pi])$-function ξ_n depend only on n, T_1 and T_0 such that

$$\operatorname{Tr} \left\{ \phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s) \right\} = \int_0^{2\pi} \phi^{(n)}(e^{it}) \xi_n(t) dt. \tag{4.22}$$

The following lemma is essential to prove Theorem 4.4.1.

Lemma 4.4.2. *Assume notations and hypotheses of the above Theorem 4.4.1. Let $T := U_{T_1,T_0}, V := U_{T_0}$ and $\mathscr{F} = \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})$. Let*

$$\begin{aligned} X_0 :&= T^n - V^n, Y_0 := T_1^n - T_0^n, \\ X_r :&= V^{\alpha_0} P_{\mathscr{F}} \left((iM)^{l_1} V\right) V^{\alpha_1} \cdots P_{\mathscr{F}} \left((iM)^{l_r} V\right) V^{\alpha_r}, \\ Y_r :&= T_0{}^{\alpha_0} P_{\mathcal{H}} \left((iM)^{l_1} W\right) T_0{}^{\alpha_1} \cdots P_{\mathcal{H}} \left((iM)^{l_r} W\right) T_0{}^{\alpha_r}, \end{aligned}$$

where the operators M, W are given in (4.30) and (4.34) respectively, $\alpha_j \geq 0$ for $0 \leq j \leq r$, and $l_{j'} \geq 1$ for $1 \leq j' \leq r$, and $r \geq 1$. Then for each integer $r \geq 0$,

(i) $P_{\mathcal{H}} X_r\Big|_{\mathcal{H}} = Y_r$, and

(ii) $P_{\mathscr{F} \ominus \mathcal{H}} X_r\Big|_{\mathscr{F} \ominus \mathcal{H}} = P_{\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})} X_r P_{\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})}\Big|_{\mathscr{F} \ominus \mathcal{H}}$.

Proof. For $r = 0$, it follows from the structures of T, and V that

$$P_{\mathcal{H}} X_r\Big|_{\mathcal{H}} = Y_r \tag{4.23}$$

For $r \geq 1$, to show $P_{\mathcal{H}} X_r\Big|_{\mathcal{H}} = Y_r$, we require the block matrix representations of M^n and V^n on the space $\mathscr{F} \oplus \mathcal{D}_T := \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathcal{D}_{T_0} \oplus S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \oplus \mathcal{D}_{T_1}$ for any $n \in \mathbb{N}$ and they are the following:

$$M^n = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & * \\ 0 & * & * & 0 & * \\ 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & * \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}, \tag{4.24}$$

and

$$\begin{aligned} V^n &= \begin{bmatrix} S^{*n}_{\mathcal{D}_{T_0^*}} & 0 & 0 \\ * & T_0^n & 0 \\ * & L_n & S^n_{\mathcal{D}_{T_0}} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \end{bmatrix} \\ &= \begin{bmatrix} S^{*n}_{\mathcal{D}_{T_0^*}} & 0 & 0 & 0 & 0 \\ * & T_0^n & 0 & 0 & 0 \\ * & D_{T_0} T_0^{n-1} & 0 & 0 & 0 \\ * & * & S^n_{\mathcal{D}_{T_0}} & S^n_{\mathcal{D}_{T_0}} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}, \end{aligned} \tag{4.25}$$

where $*$ stands for some non-zero entries and $L_n = D_{T_0} T_0^{n-1} + S_{\mathcal{D}_{T_0}} L_{n-1}, L_0 = 0, n \geq 1$. Therefore using the structures (4.24) and (4.25) of M^n and V^n respectively we conclude that

$$\begin{aligned} P_{\mathcal{H}} X_2\Big|_{\mathcal{H}} &= P_{\mathcal{H}} V^{\alpha_0} P_{\mathscr{F}}((iM)^{l_1} V) V^{\alpha_1} P_{\mathscr{F}}((iM)^{l_2} V) V^{\alpha_2}\Big|_{\mathcal{H}} \\ &= P_{\mathcal{H}} V^{\alpha_0} P_{\mathcal{H} \oplus \mathcal{D}_{T_0}}((iM)^{l_1} P^{\perp}_{S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})} V) V^{\alpha_1} P_{\mathcal{H} \oplus \mathcal{D}_{T_0}}((iM)^{l_2} P^{\perp}_{S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})} V) V^{\alpha_2}\Big|_{\mathcal{H}} \\ &= P_{\mathcal{H}} V^{\alpha_0} P_{\mathcal{H}}((iM)^{l_1} P^{\perp}_{S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})} V) V^{\alpha_1} P_{\mathcal{H}}((iM)^{l_2} P^{\perp}_{S_{\mathcal{D}_{T_0}} \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})} V) V^{\alpha_2}\Big|_{\mathcal{H}} \\ &= T_0^{\alpha_0} P_{\mathcal{H}}((iM)^{l_1} W) T_0^{\alpha_1} P_{\mathcal{H}}((iM)^{l_2} W) T_0^{\alpha_2} = Y_2, \end{aligned} \tag{4.26}$$

and similarly for $r \geq 3$ we have

$$P_{\mathcal{H}} X_r\Big|_{\mathcal{H}} = T_0{}^{\alpha_0} P_{\mathcal{H}} \left((iM)^{l_1} W\right) T_0{}^{\alpha_1} \cdots P_{\mathcal{H}} \left((iM)^{l_r} W\right) T_0{}^{\alpha_r} = Y_r. \tag{4.27}$$

Note that for $r = 0, 1$, it was mentioned in the proof of [40, Theorem 2.3], that

$$P_{\mathscr{F} \ominus \mathcal{H}} X_r\Big|_{\mathscr{F} \ominus \mathcal{H}} = P_{\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})} X_r P_{\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})}\Big|_{\mathscr{F} \ominus \mathcal{H}},$$

For $r \geq 2$, analyzing the structures of M^n and V^n as in (4.24) and (4.25) respectively we conclude that

$$\begin{aligned}
&P_{\mathscr{F}\ominus\mathcal{H}}X_r\Big|_{\mathscr{F}\ominus\mathcal{H}} \\
=&P_{\mathscr{F}\ominus\mathcal{H}}V^{\alpha_0}P_{\mathscr{F}}((iM)^{l_1}V)V^{\alpha_1}\cdots P_{\mathscr{F}}((iM)^{l_{r-1}}V)V^{\alpha_{r-1}}P_{\mathscr{F}}((iM)^{l_r}V)V^{\alpha_r}\Big|_{\mathscr{F}\ominus\mathcal{H}} \\
=&P_{\mathscr{F}\ominus\mathcal{H}}V^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}\cdot\cdot P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V) \\
&\qquad\times V^{\alpha_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_r}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_r}\Big|_{\mathscr{F}\ominus\mathcal{H}} \\
=&P_{\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})}V^{\alpha_0}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_1}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}\cdot\cdot P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V) \\
&\qquad\times V^{\alpha_{r-1}}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}((iM)^{l_r}P_{\mathcal{H}\oplus\mathcal{D}_{T_0}}V)V^{\alpha_r}P_{\mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D})}\Big|_{\mathscr{F}\ominus\mathcal{H}}.
\end{aligned} \tag{4.28}$$

This complete the proof. □

Proof of Theorem 4.4.1. Following the steps of the proof of [40, Theorem 2.3], we first dilate T_0 to its minimal unitary dilation $V := U_{T_0}$ on $\mathscr{F} = \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})$, and then extend contraction T_1 to the contraction $T := U_{T_1,T_0}$ on $\mathscr{F} = \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D})$. Now to apply our previous theorem, that is Theorem 4.3.2, we dilate T to its minimal dilation $U_1 := U_T$ on $\mathcal{K} = \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \oplus (\mathscr{F} \oplus \mathcal{D}_T) \oplus S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D})$ and extend V to the unitary $U_0 := U_{V,T}$ on $\mathcal{K}$. Finally, following similar lines of argument of the proof of [40, Theorem 2.3], we conclude that there exists a self-adjoint operator $A \in \mathcal{B}_n(\mathcal{K})$ such that $U_1 = e^{iA}U_0$ with the block matrix representation

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathscr{F} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T^*}}(\mathbb{D}) \\ \mathscr{F} \oplus \mathcal{D}_T \\ S_{\mathcal{D}_T}\mathbf{H}^2_{\mathcal{D}_T}(\mathbb{D}) \end{bmatrix}, \tag{4.29}$$

where

$$M = \begin{bmatrix} I & 0 & 0 & 0 & 0 \\ 0 & T_1T_0^* & T_1D_{T_0} & 0 & -D_{T_1^*}V_{T_1} \\ 0 & -V_{T_0}^*D_{T_0^*} & |T_0| & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ 0 & D_{T_1}T_0^* & D_{T_1}D_{T_0} & 0 & T_1^*V_{T_1} \end{bmatrix} : \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix} \to \begin{bmatrix} \mathbf{H}^2_{\mathcal{D}_{T_0^*}}(\mathbb{D}) \\ \mathcal{H} \\ \mathcal{D}_{T_0} \\ S_{\mathcal{D}_{T_0}}\mathbf{H}^2_{\mathcal{D}_{T_0}}(\mathbb{D}) \\ \mathcal{D}_{T_1} \end{bmatrix}. \tag{4.30}$$

Therefore applying Theorem 4.3.2 corresponding to the pair (T, V) we conclude that for $\phi \in$

$\mathcal{F}_n(\mathbb{T})$,

$$\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(V_s)\right\} \in \mathcal{B}_1(\mathcal{H}), \tag{4.31}$$

and there exists an $L^1([0, 2\pi])$-function ξ_n depend only on n, T and V such that

$$\operatorname{Tr}\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(V_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it})\xi_n(t)dt, \tag{4.32}$$

where $V_s = P_{\mathscr{F}} e^{isM} V$, $s \in [0, 1]$. Our next aim is to show that for $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\operatorname{Tr}\left\{\phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s)\right\} = \operatorname{Tr}\left\{\phi(T) - \phi(V) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(V_s)\right\}, \tag{4.33}$$

where

$$T_s = P_{\mathcal{H}} V_s\Big|_{\mathcal{H}} = P_{\mathcal{H}} e^{isB} \begin{bmatrix} 0 \\ T_0 \\ D_{T_0} \\ 0 \end{bmatrix} = P_{\mathcal{H}} e^{isM} W, \quad \text{where} \quad W := V\Big|_{\mathcal{H}} = \begin{bmatrix} 0 \\ T_0 \\ D_{T_0} \\ 0 \end{bmatrix}, \tag{4.34}$$

is a bounded operator from $\mathcal{H}$ to $\mathscr{F} \oplus \mathcal{D}_T$. Using Lemma 4.3.1 and Lemma 4.4.2 along with the similar type of arguments mentioned in the proof of Theorem 4.3.2, we conclude the identity (4.33). Thus the conclusion of the theorem follows by combining equations (4.32) and (4.33). This completes the proof.

□

Remark 4.4.3. *By [66, Theorem 4.4], and similar lines of proof of Theorem 4.4.1, it follows that the above trace formula (4.22) also holds for the class $\mathcal{F}_n(\mathbb{T})$.*

4.5 Higher-order Trace formula for pair of maximal dissipative operators

In this section, our main aim is to prove the trace formula for pairs of maximal dissipative operators as an application of our main theorem in the previous section. Recall that the Cayley transform of a maximal dissipative operator (see Lemma 1.2.12) A is a contraction $T : \mathcal{H} \to \mathcal{H}$

given by $T = (i-A)(i+A)^{-1}$ such that $\ker T = \ker(i-A)$ and $\ker T^* = \ker(i+A^*)$. Furthermore, if $\text{Dom}(A) = \text{Dom}(A^*)$, then

$$D_T = 2|(\text{Im}A)^{1/2}(i+A)^{-1}|, \quad D_{T^*} = 2|(\text{Im}A)^{1/2}(i-A^*)^{-1}|, \tag{4.35}$$

$$\mathcal{D}_T = \overline{((i-A^*)^{-1}(\text{Im}A)\text{Dom}(A))}, \quad \mathcal{D}_{T^*} = \overline{((i+A)^{-1}(\text{Im}A)\text{Dom}(A))}. \tag{4.36}$$

Let $\psi \in \mathcal{F}^+_{nn}(\mathbb{R})$, then $\psi(\lambda) = \phi\left(\frac{i-\lambda}{i+\lambda}\right)$ for some $\phi \in \mathcal{F}^+_{nn}(\mathbb{T})$. Now we set

$$\psi(A) = \phi(T).$$

The following lemma is essential to prove the main theorem in this section.

Lemma 4.5.1. *Let $\psi \in \mathcal{F}^+_{nn}(\mathbb{R})$ be such that $\psi(\lambda) = \phi\left(\frac{i-\lambda}{i+\lambda}\right)$ for some $\phi \in \mathcal{F}_n(\mathbb{T})$. Now if we substitute $z = e^{it} = \frac{i-\lambda}{i+\lambda}$, then $\phi(z) = \phi(e^{it}) = \psi(\lambda)$, $\lambda = \tan\frac{t}{2}$, and for all $1 \le q \le n$,*

$$\phi^{(q)}(z) = \left(\sum_{k=0}^{q-1} p_{k,q}(\lambda)\ \psi^{(q-k)}(\lambda)\right)\frac{d\lambda}{dz}, \tag{4.37}$$

where $p_{k,q}$ are polynomials in λ of degree $(2(q-1)-k)$ and it is given recursively as follows

$p_{0,1}(\lambda) = 1$ and for $q \ge 2$

$$p_{k,q}(\lambda) = \begin{cases} (i/2)(i+\lambda)^2\ p_{0,q-1}(\lambda) & \text{for } k=0,\\ (i/2)\left\{(i+\lambda)^2\left(p_{k,q-1}(\lambda)+p^{(1)}_{k-1,q-1}(\lambda)\right)+2(i+\lambda)p_{k-1,q-1}(\lambda)\right\} & \text{for } 1\le k\le q-2,\\ (i/2)\left[(i+\lambda)^2 p^{(1)}_{q-2,q-1}(\lambda)+2(i+\lambda)p_{q-2,q-1}(\lambda)\right] & \text{for } k=q-1.\end{cases}$$

Proof. We prove the identity (4.37) by principle of mathematical induction. For $q=1$, $\phi^{(1)}(z) = \psi^{(1)}(\lambda)\frac{d\lambda}{dz}$ and hence (4.37) is true for $q=1$. Suppose (4.37) is true for $q = m \le n-1$, that is

$$\phi^{(m)}(z) = \left(\sum_{k=0}^{m-1} p_{k,m}(\lambda)\psi^{(m-k)}(\lambda)\right)\frac{d\lambda}{dz}.$$

Now we will show that (4.37) is also true for $q = m+1$. Note that

$$\begin{aligned}\phi^{(m+1)}(z) &= \sum_{k=0}^{m-1}\left[\left(p^{(1)}_{k,m}(\lambda)\psi^{(m-k)}(\lambda)+p_{k,m}(\lambda)\psi^{(m+1-k)}(\lambda)\right)\frac{d\lambda}{dz}+i(i+\lambda)p_{k,m}(\lambda)\psi^{(m-k)}(\lambda)\right]\frac{d\lambda}{dz}\\ &= p_{0,m}(\lambda)\psi^{(m+1)}(\lambda)\left(\frac{d\lambda}{dz}\right)^2+\sum_{k=0}^{m-2}\left[p_{k+1,m}(\lambda)\frac{d\lambda}{dz}+p^{(1)}_{k,m}(\lambda)\frac{d\lambda}{dz}+i(i+\lambda)p_{k,m}(\lambda)\right]\end{aligned}$$

$$\times \psi^{(m-k)}(\lambda)\frac{d\lambda}{dz} + \left[p^{(1)}_{m-1,m}(\lambda)\frac{d\lambda}{dz} + i(i+\lambda)p_{m-1,m}(\lambda)\right]\psi^{(1)}(\lambda)\frac{d\lambda}{dz}$$
$$= p_{0,m}(\lambda)\psi^{(m+1)}(\lambda)\left(\frac{d\lambda}{dz}\right)^2 + \sum_{k=1}^{m-1}\left[p_{k,m}(\lambda)\frac{d\lambda}{dz} + p^{(1)}_{k-1,m}(\lambda)\frac{d\lambda}{dz} + i(i+\lambda)p_{k-1,m}(\lambda)\right]$$
$$\times \psi^{(m+1-k)}(\lambda)\frac{d\lambda}{dz} + \left[p^{(1)}_{m-1,m}(\lambda)\frac{d\lambda}{dz} + i(i+\lambda)p_{m-1,m}(\lambda)\right]\psi^{(1)}(\lambda)\frac{d\lambda}{dz}$$
$$= \left(\sum_{k=0}^{m} p_{k,m+1}(\lambda)\psi^{(m+1-k)}(\lambda)\right)\frac{d\lambda}{dz},$$

where

$$p_{k,m+1}(\lambda) = \begin{cases} (i/2)(i+\lambda)^2\, p_{0,m}(\lambda) & \text{for } k=0,\\ (i/2)\left\{(i+\lambda)^2\left(p_{k,m}(\lambda) + p^{(1)}_{k-1,m}(\lambda)\right) + 2(i+\lambda)p_{k-1,m}(\lambda)\right\} & \text{for } 1\le k\le m-1,\\ (i/2)\left[(i+\lambda)^2 p^{(1)}_{m-1,m}(\lambda) + 2(i+\lambda)p_{m-1,m}(\lambda)\right] & \text{for } k=m,\end{cases}$$

and degree of $p_{k,m+1}$ is $(2((m+1)-1)-k)$, and hence (4.37) is true for $q=m+1$. Therefore the result follows by principle of mathematical induction. This completes the proof. □

Now we are in a position to state and prove our main result in this section. It is important to note that we make the hypothesis of our next theorem in such a way so that we can apply Theorem 4.4.1 to achieve our goal.

Theorem 4.5.2. *Let $n\in\mathbb{N}$, $n\ge 2$. Let A_0 and A_1 be two maximal dissipative operators on $\mathcal{H}$ such that*

(*i*) $\dim\ker(A_j - i) = \dim\ker(A_j^* + i)$, *for* $j=0,1$,

(*ii*) $(A_1+i)^{-1} - (A_0+i)^{-1} \in \mathcal{B}_n(\mathcal{H})$, *and*

(*iii*) $\operatorname{Im} A_j = \dfrac{A_j - A_j^*}{2i} \in \mathcal{B}_{n/2}(\mathcal{H})$ *for* $j=0,1$.

Let $T_0 = (i-A_0)(i+A_0)^{-1}$ and $T_1 = (i-A_1)(i+A_1)^{-1}$ be the corresponding contractions obtained by the Cayley transform of maximal dissipative operators A_0 and A_1 respectively. Set $A_s = \left(2i(1-T_s)^{-1} - i\right)$, where T_s as in (4.21). Then for $\psi\in\mathcal{F}^+_{nn}(\mathbb{R})$,

$$\left\{\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\bigg|_{s=0}\psi(A_s)\right\} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists an $L^1(\mathbb{R},(1+\lambda^2)^{-1}d\lambda)$-function η_n depend only on n, A_1 and A_0 such that

$$\operatorname{Tr}\left\{\psi(A_1) - \psi(A_0) - \sum_{k=1}^{n-1}\frac{1}{k!}\frac{d^k}{ds^k}\bigg|_{s=0}\psi(A_s)\right\} = \int_{-\infty}^{\infty}\left(\sum_{k=0}^{n-1}p_{k,n}(\lambda)\psi^{(n-k)}(\lambda)\right)\eta_n(\lambda)d\lambda,$$

where $\psi(\lambda) = \phi\left(\frac{i-\lambda}{i+\lambda}\right)$ *for some* $\phi \in \mathcal{F}_{nn}^{+}(\mathbb{T})$ *and* $\lambda \in \mathbb{R}$.

Proof. Let $T_j = (i - A_j)(i + A_j)^{-1}$ be the contraction obtained via the Cayley transform of a maximal dissipative operator A_j and hence $\ker T_j = \ker(i - A_j)$ and $\ker T_j^* = \ker(i + A_j^*)$ for $j = 0, 1$. Furthermore, note that

$$T_1 - T_0 = 2i\left[(i + A_1)^{-1} - (i + A_0)^{-1}\right].$$

Therefore using the hypothesis (i), (ii) and (iii) we conclude that the pair of contractions (T_0, T_1) on $\mathcal{H}$ satisfies the hypothesis (i) and (ii) of Theorem 4.4.1. Let V_j be the unitary operator on $\mathcal{H}$ such that $(i - A_j)(i + A_j)^{-1} = V_j|(i - A_j)(i + A_j)^{-1}|$ for $j = 0, 1$. Thus by applying Theorem 4.4.1 corresponding to the pair (T_0, T_1) we get for $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\left\{\phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s)\right\} \in \mathcal{B}_1(\mathcal{H}), \tag{4.38}$$

and there exists an $L^1([0, 2\pi])$-function ξ_n depend only on n, T_1 and T_0 such that

$$\operatorname{Tr}\left\{\phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it})\xi_n(t)dt, \tag{4.39}$$

where

$$T_s = P_{\mathcal{H}} e^{isM} \begin{bmatrix} 0 \\ (i - A_0)(i + A_0)^{-1} \\ |2(\mathrm{Im}A_0)^{1/2}(i + A_0)^{-1}| \\ 0 \end{bmatrix}, \quad s \in [0, 1], \tag{4.40}$$

and M is a self-adjoint operator on $\mathscr{F} \oplus \overline{((i - A_1^*)^{-1}(\mathrm{Im}A_1)\mathrm{Dom}(A_1))}$ such that

$$\mathscr{F} = \mathbf{H}^2_{\overline{((i+A_0)^{-1}(\mathrm{Im}A_0)\mathrm{Dom}(A_0))}}(\mathbb{D}) \oplus \mathcal{H} \oplus \mathbf{H}^2_{\overline{\left((i-A_0^*)^{-1}(\mathrm{Im}A_0)\mathrm{Dom}(A_0)\right)}}(\mathbb{D}),$$

$\sigma(M) \subseteq (-\pi, \pi]$, $M \in \mathcal{B}_n(\mathscr{F} \oplus \overline{((i - A_1^*)^{-1}(\mathrm{Im}A_1)\mathrm{Dom}(A_1))})$.
Now it easy to observe that for $\psi(\lambda) = \phi\left(\frac{i+\lambda}{i-\lambda}\right) \in \mathcal{R}_n$, where $\phi \in \mathcal{F}_n(\mathbb{T})$,

$$\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s) = \phi(T_1) - \phi(T_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \phi(T_s), \tag{4.41}$$

where $A_s = (i - 2i(T_s + 1)^{-1})$. Therefore using equations (4.38), (4.39) and (4.41) we conclude that

$$\left\{\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\right\} \in \mathcal{B}_1(\mathcal{H}),$$

and there exists an $L^1([0,2\pi])$-function ξ_n depend only on n, A_1 and A_0 such that

$$\operatorname{Tr}\left\{\psi(A_1) - \psi(A_0) - \sum_{k=1}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\right\} = \int_0^{2\pi} \phi^{(n)}(e^{it})\xi_n(t)dt,$$

which by applying Lemma 4.5.1 yields that

$$\operatorname{Tr}\left\{\psi(A_1) - \psi(A_0) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{ds^k}\Big|_{s=0} \psi(A_s)\right\} = \int_{-\infty}^{\infty} \left(\sum_{k=0}^{n-1} p_{k,n}(\lambda)\psi^{(n-k)}(\lambda)\right) \eta_n(\lambda)d\lambda, \quad (4.42)$$

where $\eta_n(\lambda) = \xi_n(t) = i(i+\lambda)(\lambda - i)^{-1}\xi_n(2\tan^{-1}(\lambda))$ and $\eta_n \in L^1\left(\mathbb{R}, (1+\lambda^2)^{-1}d\lambda\right)$. This completes the proof. □

CHAPTER 5

Approximation of the spectral action functional in the case of compact resolvents

5.1 Introduction

Let H_0 be a closed densely defined self-adjoint operator in $\mathcal{H}$ and assume that its resolvent is compact. Examples of such operators include differential operators on compact Riemannian manifolds (see, e.g., [7, Chapter 3, Section B] or [29, Chapter 3, Section 6]) and generalized Dirac operators of unital spectral triples (see, e.g., [71]). For a sufficiently nice function f and a bounded self-adjoint operator on $\mathcal{H}$, which models a gauge potential, we consider a spectral action functional $V \mapsto \mathrm{Tr}(f(H_0+V))$. The latter was introduced in [15] to encompass different field actions in noncommutative geometry and recently received considerable attention in the literature. Counterparts of the spectral action functional also arise in problems of mathematical physics on deterministic and random Dirac and Schrödinger operators (see, e.g., [68, 69]).

A perturbation approach to the spectral action functional was taken in [72], where a non-commutative analog of the Taylor series expansion served as a starting point to understanding the structure of gauge fluctuations. Analytical aspects of Taylor approximations of the spectral action functional were also studied in [65, 67]. In this chapter we significantly relax assumptions imposed on admissible functions f in [65, 67]. We note that it is important to relax assumptions on f appearing in the spectral action since that function might be prescribed by the model [16].

Given a natural number $n \in \mathbb{N}$ and suitable f and H_0, we denote the n-th order Taylor remainder of the spectral action functional $V \mapsto \operatorname{Tr}\big(f(H_0+V)\big)$ by

$$\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right) = \operatorname{Tr}\Big(f(H_0+V) - f(H_0) - \sum_{k=1}^{n-1} \frac{1}{k!}\frac{d^k}{ds^k} f(H_0+sV)\big|_{s=0}\Big). \tag{5.1}$$

In Theorem 5.3.1 we establish that

$$\left|\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right)\right| \le D_{a,b,n,\epsilon,H_0,V}\|f^{(n)}\|_\infty \tag{5.2}$$

for every H_0 with compact resolvent and every n-times differentiable compactly supported in (a,b) function f with bounded $f^{(n)}$ and we derive an upper bound on the constant $D_{a,b,n,\epsilon,H_0,V}$ revealing explicit dependence on $H_0, V, n, a, b, \epsilon$. We also establish the trace formula

$$\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right) = \int_{\mathbb{R}} f^{(n)}(\lambda)\eta_{n,H_0,V}(\lambda)d\lambda \tag{5.3}$$

for every n-times differentiable compactly supported in (a,b) function f such that $f^{(n)}$ exists almost everywhere and $f^{(n)} \in L^2(\mathbb{R})$. The real-valued function $\eta_{n,H_0,V} \in L^1((a,b))$ is determined by (5.3) uniquely up to a polynomial summand of degree at most $n-1$.

In Theorem 5.4.7 we relax the differentiability assumption and remove the support restriction on functions f satisfying (5.3) under the stronger assumption on the operator H_0. Namely, in the case when $(H_0 - iI)^{-1}$ belongs to the Schatten ideal, we establish (5.3) for $(n-1)$-times continuously differentiable functions with suitable decay at infinity. The locally integrable real-valued function $\eta_{n,H_0,V}$ is determined by (5.3) uniquely up to a polynomial summand of degree at most $n-1$ and it satisfies the estimate

$$|\eta_n(x)| \le \ \text{const}_n\,(2+\|V\|)\,\|V\|^{n-1}\,\|(H_0-iI)^{-1}\|_n^n\,(1+|x|)^n$$

for every $x \in \mathbb{R}$, where $\|\cdot\|$ denotes the operator norm and $\|\cdot\|_n$ the Schatten n-norm.

Our bound (5.2) extends the analogous bound of [67], where the additional assumption $f \in C_c^{n+1}((a,b))$ was imposed. The formula (5.3) was earlier established under the additional restriction $f \in C^3((a,b))$ in the case $n=1$ in [6, Theorem 2.5] and under the restriction $f \in C_c^{n+1}((a,b))$ in the case $n \ge 2$ in [67]. Other results in this direction were obtained in [73, Theorem 18 and Corollary 19] and [65, Theorems 3.4 and 3.10]. The result of Theorem 5.4.7 relaxes the differentiability assumption made in [71, Theorem 4.1].

The chapter is organized as follows: preliminary results are discussed in Section 5.2; our main results are proved in Section 5.3 and Section 5.4 under the assumptions that H_0 has compact resolvent and that the resolvent of H_0 belongs to the Schatten n-class, respectively.

5.2 Preliminaries and notation

We denote positive constants by letters c, d, C, D with subscripts indicating dependence on their parameters. For instance, the symbol c_α denotes a constant depending only on the parameter α.

Given $f \in L^1(\mathbb{R})$, let $\hat{f}$ denote the Fourier transform of f. We will use the well-known property that every $f \in C_c^n(\mathbb{R})$ satisfies $\widehat{f^{(n-1)}} \in L^1(\mathbb{R})$.

We will need the following elementary lemma.

Lemma 5.2.1. *Let $a, b \in \mathbb{R}$, $a < b$, $k \in \mathbb{N}$, and $f \in D_c^k((a,b))$ be such that $f^{(k)} \in B([a,b])$. Then,*

$$\|f^{(j)}\|_\infty \leq (b-a)^{k-j}\|f^{(k)}\|_\infty, \quad j = 0, \ldots, k.$$

Proof. By using the following identity, we conclude the proof.

$$f(x) - f(a) = \int_a^x f'(t)dt.$$

□

Operators with compact resolvent. Let $\mathcal{H}$ be a fix complex separable Hilbert space. When H is a closed densely defined self-adjoint operator in $\mathcal{H}$, we briefly write that H *is a self-adjoint operator in* $\mathcal{H}$. We say that a self-adjoint operator H in $\mathcal{H}$ *has compact resolvent* $(H - zI)^{-1}$ is compact for some and, hence, for each resolvent point z of H.

The following useful property is a consequence of the second resolvent identity (see, e.g., [6, Lemma 1.3]).

Lemma 5.2.2. *Let H_0 be a self-adjoint operator in $\mathcal{H}$ with compact resolvent and let V be a bounded self-adjoint operator on $\mathcal{H}$. Then, $H = H_0 + V$ also has compact resolvent.*

Proof. The result follows from the resolvent identity

$$(H_0 + V - i)^{-1} - (H_0 - i)^{-1} = (H_0 - i)^{-1} V (H_0 + V - i)^{-1}$$

□

Let $E_H(\cdot)$ denote the spectral measure of a self-adjoint operator H. The following result is a consequence of Lemma 5.2.2 and [6, Lemma 1.4].

Lemma 5.2.3. *Let H_0 be a self-adjoint operator in $\mathcal{H}$ with compact resolvent and let V be a bounded self-adjoint operator on $\mathcal{H}$. Then, for every compact subset $\Delta \subset \mathbb{R}$, the spectral projections $E_{H_0}(\Delta)$ and $E_{H_0+V}(\Delta)$ are finite rank operators.*

Proof. Let H_0 be a self-adjoint operator in $\mathcal{H}$ having compact resolvent, $V \in \mathcal{B}_{sa}(\mathcal{H})$ and $H = H_0 + V$. Then by [14, Appendix B, Lemma 6] we have

$$(1 + H^2)^{-1} \leq \; (1 + \|V\| + \|V\|^2)(1 + H_0^2)^{-1}. \tag{5.4}$$

Let $h \in \mathcal{H}$ and Δ is compact subset of $\mathbb{R}$, then

$$\begin{aligned} \langle (1 + H^2)^{-1} h, h \rangle &= \int_{\mathbb{R}} (1 + \lambda^2)^{-1} \; d\|E_H(\lambda)h\|^2 \\ &\geq \int_{\Delta} (1 + \lambda^2)^{-1} \; d\|E_H(\lambda)h\|^2 \\ &\geq \int_{\Delta} (1 + \max_{\lambda \in \Delta} \lambda^2)^{-1} d\|E_H(\lambda)h\|^2 \\ &= (1 + \max_{\lambda \in \Delta} \lambda^2)^{-1} \|E_H(\Delta)h\|^2. \end{aligned} \tag{5.5}$$

Therefore from 5.4 and 5.5 we have

$$E_H(\Delta) \leq (1 + \max_{\lambda \in \Delta} \lambda^2)(1 + \|V\| + \|V\|^2)(1 + H_0^2)^{-1},$$

which implies that $E_H(\Delta)$ is a compact operator as $(1 + H_0^2)^{-1}$ is compact and hence $E(\Delta)$ is a finite rank operator. □

Let $f \in C^n(\mathbb{R})$. Recall that the divided difference of order n is an operation on the function f of one (real) variable, and is defined recursively as follows:

$$f^{[0]}(\lambda) = f(\lambda),$$

$$f^{[n]}(\lambda_0, \lambda_1, \ldots, \lambda_n) = \begin{cases} \frac{f^{[n-1]}(\lambda_0, \lambda_1, \ldots, \lambda_{n-2}, \lambda_n) - f^{[n-1]}(\lambda_0, \lambda_1, \ldots, \lambda_{n-2}, \lambda_{n-1})}{\lambda_n - \lambda_{n-1}} & \text{if} \quad \lambda_n \neq \lambda_{n-1}, \\ \frac{\partial}{\partial \lambda} f^{[n-1]}(\lambda_0, \lambda_1, \ldots, \lambda_{n-2}, \lambda)\big|_{\lambda = \lambda_{n-1}} & \text{if} \quad \lambda_n = \lambda_{n-1}. \end{cases}$$

Multilinear operator integrals. Let H be a self-adjoint operator in $\mathcal{H}$ and let $f \in C^n(\mathbb{R})$ be such that $\widehat{f^{(n)}} \in L^1(\mathbb{R})$. Let $p_k \in [1, \infty], 1 \leq k \leq n$, and $E_{l,m} = E_H\big(\big[\frac{l}{m}, \frac{l+1}{m}\big)\big)$ for $m \in \mathbb{N}$ and $l \in \mathbb{Z}$. Define a multilinear map on $\mathcal{B}_{p_1}(\mathcal{H}) \times \cdots \times \mathcal{B}_{p_n}(\mathcal{H})$ by

$$T^{H,\ldots,H}_{f^{[n]}}(V_1, V_2, \ldots, V_n) \tag{5.6}$$
$$= \lim_{m\to\infty} \lim_{N\to\infty} \sum_{|l_0|,|l_1|,\ldots,|l_n|\leq N} f^{[n]}\Big(\frac{l_0}{m}, \frac{l_1}{m}, \ldots, \frac{l_n}{m}\Big) E_{l_0,m} V_1 E_{l_1,m} V_2 E_{l_2,m} \cdots V_n E_{l_n,m},$$

where the limits are evaluated in the norm $\|\cdot\|_p$, $\frac{1}{p} = \frac{1}{p_1} + \frac{1}{p_2} + \cdots + \frac{1}{p_n}$. The existence of the limits in (5.6) is justified in [52, Lemma 3.5]. We call $T^{H,\ldots,H}_{f^{[n]}}$ defined in (5.6) a *multilinear operator integral with symbol* $f^{[n]}$ and write $T_{f^{[n]}}$ when there is no ambiguity which element H is used.

Discussion of multiple operator integrals, including those with more general symbols, and their applications can be found in [69]. It was shown in [65, Lemma 3.1, Theorem 3.2] that the multilinear operator integral given by (5.6) is bounded for all $f \in C_c^{n+1}(\mathbb{R})$ when H has compact resolvent.

The following estimate is a consequence of [52, Theorem 5.3 and Remark 5.4] and [69, Theorem 4.4.7].

Theorem 5.2.4. *Let $k \in \mathbb{N}$ and let $\alpha, \alpha_1, \ldots, \alpha_k \in (1, \infty)$ satisfy $\frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_k} = \frac{1}{\alpha}$. Let H and $\tilde{H}$ be two self-adjoint operators in $\mathcal{H}$. Assume that $V_\ell \in \mathcal{B}_{\alpha_\ell}(\mathcal{H})$, $1 \leq \ell \leq k$. Then there exists $c_{\alpha,k} > 0$ such that*

$$\|T^{\tilde{H},H,\ldots,H}_{f^{[k]}}(V_1, V_2, \ldots, V_k)\|_\alpha \leq c_{\alpha,k} \|f^{(k)}\|_\infty \prod_{1\leq\ell\leq k} \|V_\ell\|_{\alpha_\ell} \tag{5.7}$$

for every $f \in C_b^k(\mathbb{R})$.

We also have the following bound for the seminorm $|\operatorname{Tr}(\cdot)|$ of a multilinear operator integral.

Theorem 5.2.5. *Let $k \in \mathbb{N}$ and let $\alpha_1, \ldots, \alpha_k \in (1, \infty)$ satisfy $\frac{1}{\alpha_1} + \cdots + \frac{1}{\alpha_k} = 1$. Let H be a self-adjoint operator in $\mathcal{H}$. Assume that $V_\ell \in \mathcal{B}_{\alpha_\ell}(\mathcal{H})$, $1 \leq \ell \leq k$. Then, for $c_{1,k} > 0$ satisfying* (5.7),

$$|\operatorname{Tr}(T^{H,H,\ldots,H}_{f^{[k]}}(V_1, \ldots, V_k))| \leq c_{1,k} \|f^{(k)}\|_\infty \prod_{1\leq\ell\leq k} \|V_\ell\|_{\alpha_\ell} \tag{5.8}$$

for every f with $f^{(k)} \in C_0(\mathbb{R})$ satisfying $\widehat{f^{(k)}} \in L^1(\mathbb{R})$.

Proof. By the definition of the multiple operator integral (5.6) and cyclicity of the trace,

$$\operatorname{Tr}\left(T^{H,H,\dots,H}_{f^{[k]}}(V_1,\dots,V_k)\right) = \operatorname{Tr}\left(T^{H,H,\dots,H}_{\tilde{f}^{[k]}}(V_1,\dots,V_{k-1})V_k\right), \tag{5.9}$$

where $\tilde{f}^{[k]}(\lambda_0,\lambda_1,\dots,\lambda_{k-1}) = f^{[k]}(\lambda_0,\lambda_1,\dots,\lambda_{k-1},\lambda_{k-1})$. Therefore, by Hölder's inequality, Theorem 5.2.4, and [52, Remark 5.4] applied to (5.9), we obtain (5.8). □

Let $a,b\in\mathbb{R}$, $a<b$, and $\epsilon>0$. Let $a_\epsilon = a-\epsilon$, $b_\epsilon = b+\epsilon$. Define the function Φ_ϵ on $\mathbb{R}$ by

$$\Phi_\epsilon(x) = (h_1(x) - h_2(x))^4, \tag{5.10}$$

where

$$h_1(x) = \frac{\int_{a_\epsilon}^{x} \Phi(t-a_\epsilon)\Phi(a-t)\,dt}{\int_{a_\epsilon}^{a} \Phi(t-a_\epsilon)\Phi(a-t)\,dt}, \quad h_2(x) = \frac{\int_{b}^{x} \Phi(t-b)\Phi(b_\epsilon-t)\,dt}{\int_{b}^{b_\epsilon} \Phi(t-b)\Phi(b_\epsilon-t)\,dt},$$

$$\Phi(x) = \begin{cases} e^{-\frac{1}{x}} & \text{if } x>0,\\ 0 & \text{if } x\le 0.\end{cases}$$

Note that $\Phi_\epsilon|_{(a,b)} = 1$, $\Phi_\epsilon^{1/4}\in C_c^\infty((a_\epsilon,b_\epsilon))$ and $\|\Phi_\epsilon\|_\infty = 1$. Moreover, if H has compact resolvent, then by the spectral theorem, $\Phi_\epsilon(H)\in\mathcal{B}_1(\mathcal{H})$ and $\|\Phi_\epsilon(H)\|_1 \le \operatorname{Tr}(E_H(a_\epsilon,b_\epsilon))\|\Phi_\epsilon\|_\infty$ (see [67, Proposition 2.3]).

Theorem 5.2.6. *Let H_0 be a self-adjoint operator with compact resolvent in $\mathcal{H}$, $k\in\mathbb{N}$, and $V_1,V_2,\dots,V_k\in\mathcal{B}(\mathcal{H})$. Let $a,b\in\mathbb{R}$, $a<b$, and $\epsilon>0$. Then*

$$\left|\operatorname{Tr}\left(T^{H_0,\dots,H_0}_{f^{[k]}}(V_1,V_2,\dots,V_k)\right)\right| \le C_{a,b,k,\epsilon,H_0}\,\|f^{(k)}\|_\infty \prod_{\ell=1}^{k}\|V_\ell\| \tag{5.11}$$

for every $f\in F_c^{k+1}((a,b))$, where

$$C_{a,b,k,\epsilon,H_0} = \left[(k+1)2^k + c_{2,k}\right](b-a+1)^k(1+\operatorname{Tr}(E_{H_0}(a,b)))\times d_{k,\epsilon,H_0}, \tag{5.12}$$

where $c_{2,k}$ satisfies (5.7) and

$$d_{k,\epsilon,H_0} = \max\left\{\|\Phi_\epsilon(H_0)\|_1,\ \max_{1\le\ell\le k}\frac{1}{\ell!}\left\|\,\widehat{\Phi_\epsilon^{(\ell)}}\,\right\|_1\right\},$$

where Φ_ϵ is given by (5.10).

Proof. The proof follows along the lines of the proof of [67, Theorem 3.1]. □

Remark 5.2.7. *Note that the upper bound for* $\left|\operatorname{Tr}\left(T^{H_0,\ldots,H_0}_{f^{[k]}}(V_1,V_2,\ldots,V_k)\right)\right|$ *in* (5.11) *is stronger than the upper bound stated in [67, Theorem 3.1].*

The following result is a consequence of [69, Theorems 4.4.6 and 5.3.5].

Theorem 5.2.8. *Let* $n \in \mathbb{N}$ *and let* $f \in C^n(\mathbb{R})$ *be such that* $f^{(k)}, \widehat{f^{(k)}} \in L^1(\mathbb{R})$, $k = 0,1,\ldots,n$. *Let* H *be a self-adjoint operator in* $\mathcal{H}$ *with compact resolvent and let* V *be a bounded self-adjoint operator on* $\mathcal{H}$. *Then, the Gâteaux derivative* $\frac{d^k}{dt^k} f(H+tV)|_{t=0}$ *exists in the uniform operator topology and admits the multiple operator integral representation*

$$\frac{1}{k!}\frac{d^k}{ds^k} f(H+sV)\big|_{s=t} = T^{H+tV,\ldots,H+tV}_{f^{[k]}}(V,V,\ldots,V), \quad 1 \le k \le n. \tag{5.13}$$

Moreover, if $V \in \mathcal{B}_k(\mathcal{H})$, *then the above* k*-th derivative is an element in* $\mathcal{B}_1(\mathcal{H})$.

5.3 Trace formulas for operators with compact resolvents

In this section we establish our first main result.

Theorem 5.3.1. *Let* H_0 *be a self-adjoint operator in* $\mathcal{H}$ *with compact resolvent,* V *a bounded self-adjoint operator on* $\mathcal{H}$, $n \in \mathbb{N}$, *and let* $-\infty < a < b < \infty$, $\epsilon > 0$. *Then,*

$$\left|\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right)\right| \le D_{a,b,n,\epsilon,H_0,V}\|f^{(n)}\|_\infty \tag{5.14}$$

for every $f \in D^n_c((a,b))$ *with* $f^{(n)} \in B([a,b])$, *where*

$$\begin{aligned} &D_{a,b,n,\epsilon,H_0,V} \\ &= (b-a)^n \max\left\{\operatorname{Tr}(E_{H_0}([a,b])), \operatorname{Tr}(E_{H_0+V}([a,b]))\right\} + \sum_{k=1}^{n-1}(b-a)^{n-k} C_{a,b,k,\epsilon,H_0}\|V\|^k, \end{aligned} \tag{5.15}$$

and C_{a,b,k,ϵ,H_0} *satisfies* (5.11). *Furthermore, there exists a real-valued function* $\eta_{a,b,n,\epsilon,H_0,V} \in L^1((a,b))$ *such that*

$$\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right) = \int_a^b f^{(n)}(\lambda)\eta_{a,b,n,\epsilon,H_0,V}(\lambda)d\lambda \tag{5.16}$$

for every $f \in F^n_c((a,b))$ *and*

$$\int_a^b \left|\eta_{a,b,n,\epsilon,H_0,V}(\lambda)\right| d\lambda \le D_{a,b,n,\epsilon,H_0,V}. \tag{5.17}$$

The function $\eta_{a,b,n,\epsilon,H_0,V} \in L^1((a,b))$ *is determined by* (5.16) *uniquely up to a polynomial summand of degree at most* $n-1$.

Proof. By Lemma 5.2.3, $E_{H_0}([a,b])$ and $E_{H_0+V}([a,b])$ are finite projections. Let $f \in F_c^n((a,b))$.

Case 1: $n = 1$.

By the spectral theorem for a self-adjoint operator H in $\mathcal{H}$ with compact resolvent, we have

$$f(H) = f(H)E_H([a,b]) = \int_a^b f(\lambda)\, dE_H(\lambda),$$

where the integral converges in $\mathcal{B}_1(\mathcal{H})$. Hence, by continuity of the trace Tr,

$$\mathrm{Tr}\left(\mathcal{R}_{H_0,f,1}(V)\right) = \int_a^b f(\lambda) d\big(\mathrm{Tr}(E_{H_0+V}(\lambda)) - \mathrm{Tr}(E_{H_0}(\lambda))\big). \tag{5.18}$$

Integrating by parts on the right-hand side of (5.18) and applying the support property and absolute continuity of f yield

$$\begin{aligned}\mathrm{Tr}\left(\mathcal{R}_{H_0,f,1}(V)\right) &= -\int_a^b \big(\mathrm{Tr}(E_{H_0+V}([a,\lambda))) - \mathrm{Tr}(E_{H_0}([a,\lambda)))\big) df(\lambda)\\ &= \int_a^b f'(\lambda)\big(\mathrm{Tr}(E_{H_0}([a,\lambda))) - \mathrm{Tr}(E_{H_0+V}([a,\lambda)))\big) d\lambda.\end{aligned} \tag{5.19}$$

Thus, (5.16) holds for $n = 1$ with

$$\eta_{a,b,1,\epsilon,H_0,V}(\lambda) = \mathrm{Tr}(E_{H_0}([a,\lambda))) - \mathrm{Tr}(E_{H_0+V}([a,\lambda))) \tag{5.20}$$

and (5.17) holds with

$$D_{a,b,1,\epsilon,H_0,V} = (b-a) \max\big\{\mathrm{Tr}(E_{H_0}([a,b])), \mathrm{Tr}(E_{H_0+V}([a,b]))\big\}.$$

Case 2: $n \geq 2$.

By (5.19),

$$\big|\mathrm{Tr}(f(H_0+V)) - \mathrm{Tr}(f(H_0))\big| \leq \|f'\|_\infty (b-a) \max\big\{\mathrm{Tr}(E_{H_0}([a,b])), \mathrm{Tr}(E_{H_0+V}([a,b]))\big\}.$$

The latter along with Lemma 5.2.1 implies

$$\begin{aligned}&\big|\mathrm{Tr}(f(H_0+V)) - \mathrm{Tr}(f(H_0))\big|\\ &\leq \|f^{(n-1)}\|_\infty (b-a)^{n-1} \max\big\{\mathrm{Tr}(E_{H_0}([a,b])), \mathrm{Tr}(E_{H_0+V}([a,b]))\big\}.\end{aligned} \tag{5.21}$$

Combining (5.11) and (5.13) and then applying Lemma 5.2.1 yield

$$
\begin{aligned}
\left|\operatorname{Tr}\left(\frac{1}{k!}\frac{d^k}{ds^k}f(H_0+sV)\big|_{s=0}\right)\right| &\leq\ C_{a,b,k,\epsilon,H_0}\ \|f^{(k)}\|_\infty\|V\|^k\\
&\leq (b-a)^{n-k-1}C_{a,b,k,\epsilon,H_0}\|f^{(n-1)}\|_\infty\|V\|^k
\end{aligned}
\tag{5.22}
$$

for every $k=1,\dots,n-1$, where C_{a,b,k,ϵ,H_0} satisfies (5.12). Combining (5.1), (5.21), and (5.22) implies

$$
\left|\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right)\right|\leq \widetilde{D}_{a,b,n,\epsilon,H_0,V}\|f^{(n-1)}\|_\infty, \tag{5.23}
$$

where

$$
\begin{aligned}
&\widetilde{D}_{a,b,n,\epsilon,H_0,V}\\
&\quad=(b-a)^{n-1}\max\left\{\operatorname{Tr}(E_{H_0}([a,b])),\operatorname{Tr}(E_{H_0+V}([a,b]))\right\}+\sum_{k=1}^{n-1}(b-a)^{n-k-1}C_{a,b,k,\epsilon,H_0}\|V\|^k.
\end{aligned}
$$

By the Riesz representation theorem for elements in $\left(C_0(\mathbb{R})\right)^*$, Hahn-Banach theorem, and estimate (5.23), there exists a finite (complex) measure $\nu_{a,b,n,\epsilon,H_0,V}$ such that

$$
\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right)=\int_a^b f^{(n-1)}(\lambda)d\nu_{a,b,n,\epsilon,H_0,V}(\lambda) \tag{5.24}
$$

for every $f\in F_c^n((a,b))$ and the total variation of $\nu_{a,b,n,\epsilon,H_0,V}$ is bounded by

$$
\|\nu_{a,b,n,\epsilon,H_0,V}\|\leq \widetilde{D}_{a,b,n,\epsilon,H_0,V}. \tag{5.25}
$$

Integrating by parts on the right-hand side of (5.24) and applying the support property of f and absolute continuity of $f^{(n-1)}$ yield

$$
\operatorname{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right)=\int_a^b f^{(n)}(\lambda)\big(-\nu_{a,b,n,\epsilon,H_0,V}([a,\lambda))\big)d\lambda. \tag{5.26}
$$

Thus, (5.26) implies (5.16) with

$$
\eta_{a,b,n,\epsilon,H_0,V}(\lambda)=-\nu_{a,b,n,\epsilon,H_0,V}([a,\lambda)). \tag{5.27}
$$

Combining (5.25) and (5.27) ensures (5.17), where

$$
D_{a,b,n,\epsilon,H_0,V}=(b-a)\widetilde{D}_{a,b,n,\epsilon,H_0,V}. \tag{5.28}
$$

Let $\tilde{\eta}_{a,b,n,\epsilon,H_0,V}:=\operatorname{Re}\left(\eta_{a,b,n,\epsilon,H_0,V}\right)$. Since the left-hand side of (5.16) is real-valued whenever f is real-valued, we obtain that $\tilde{\eta}_{a,b,n,\epsilon,H_0,V}$ satisfies (5.16) and (5.17) for real-valued

$f \in F_c^n((a,b))$ and, consequently, for all $f \in F_c^n((a,b))$. Therefore, without loss of generality we may consider $\eta_{a,b,n,\epsilon,H_0,V}$ to be real-valued satisfying (5.16) and (5.17). Next, suppose there exists another real-valued function $\xi_{a,b,n,H_0,V} \in L^1((a,b))$ satisfying (5.16). Let $h_n = \eta_{a,b,n,\epsilon,H_0,V} - \xi_{a,b,n,H_0,V}$. Then, it follows from (5.16) that

$$\int_a^b f^{(n)}(\lambda) h_n(\lambda) d\lambda = 0 \quad \text{for all } f \in C_c^\infty((a,b)). \tag{5.29}$$

Consider the distribution T_{h_n} defined by

$$T_{h_n}(\phi) = \int_a^b \phi \, h_n \, d\lambda$$

for every $\phi \in C_c^\infty((a,b))$. By (5.29) and the definition of the derivative of a distribution, $T_{h_n}^{(n)} = 0$. Hence by [1, Theorem 3.10 and Example 2.21], h_n is a polynomial of degree at most $n-1$. Consequently, $\eta_{a,b,n,\epsilon,H_0,V} \in L^1((a,b))$ satisfying (5.16) is unique up to an additive polynomial of degree at most $n-1$.

Assume now that $n \in \mathbb{N}$ and $f \in D_c^n((a,b))$ with $f^{(n)} \in B([a,b])$. Applying Lemma 5.2.1 in (5.23) yields (5.14), completing the proof of the theorem. □

Remark 5.3.2. *It follows from the proof of Theorem 5.3.1 that the representation (5.16) with $n = 1$ holds for a larger class of functions f, namely, for every f absolutely continuous on $[a,b]$ and compactly supported in (a,b).*

Remark 5.3.3. *The uniqueness of the spectral shift function $\eta_{a,b,n,\epsilon,H_0,V}$ up to an additive polynomial of degree at most $n-1$ was not addressed in [67, Theorem 4.3].*

5.4 The case of resolvents in the Schatten n-class

In this section, we obtain an upper bound for $|\operatorname{Tr}(\mathcal{R}_{H_0,f,n}(V))|$ that is independent of the support of f under the additional assumption that the resolvent of H_0 belongs to $\mathcal{B}_n(\mathcal{H})$, $n \in \mathbb{N}$. As an application, we extend the trace formula (5.16) to a larger class of scalar functions f and obtain an entriwise bound on the spectral shift function.

The trace formula (5.3) was obtained in [71] for the class of scalar functions $\mathfrak{W}_n$ defined below under the assumption that $V(H_0 - iI)^{-1}$ belongs to the Schatten ideal $\mathcal{B}_n(\mathcal{H})$.

Definition 5.4.1. *Let $n \in \mathbb{N}$. Let $\mathfrak{W}_n$ denote the set of functions $f \in C^n(\mathbb{R})$ such that*

(i) $\widehat{f^{(k)}u^k} \in L^1(\mathbb{R})$, $k = 0, 1, \dots, n$,

(ii) $f^{(k)} \in L^1\big(\mathbb{R}, (1+|x|)^{k-1}\,dx\big)$, $k = 1, \dots, n$.

As noted in Remark 5.4.3 below, $F_c^n(\mathbb{R}) \not\subset \mathfrak{W}_n$. Our principle goal in this section is to establish the trace formula (5.1) for a larger set of functions containing $F_c^n(\mathbb{R})$. In this context, we introduce the following class of functions.

Definition 5.4.2. *Let $n \in \mathbb{N}$. Let $\mathfrak{H}_n$ denote the set of functions $f \in C^{n-1}(\mathbb{R})$ such that*

(i) $\widehat{f^{(k)}u^k}, \widehat{f^{(k)}u^{k+1}} \in L^1(\mathbb{R})$, $k = 0, 1, \dots, n-1$,

(ii) $f^{(n)}$ *exists almost everywhere,*

(iii) $f^{(k)} \in L^1\big(\mathbb{R}, (1+|x|)^{k}\,dx\big)$, $k = 0, 1, \dots, n$.

Remark 5.4.3. *We have*

$$F_c^n(\mathbb{R}) \subset \mathfrak{H}_n \subset \mathfrak{W}_{n-1}, \tag{5.30}$$

but

$$F_c^n(\mathbb{R}) \not\subset \mathfrak{W}_n, \quad \mathfrak{H}_n \not\subset \mathfrak{W}_n, \quad \mathfrak{W}_n \not\subset \mathfrak{H}_n. \tag{5.31}$$

The inclusions (5.30) follow directly from the definitions of the sets. Note that the function

$$f(x) = \begin{cases} 0 & \text{if } x < 0, \\ x^n(x-1)^n & \text{if } 0 \le x \le 1, \\ 0 & \text{if } x > 1, \end{cases}$$

satisfies $f \in F_c^n(\mathbb{R})$ but $f \notin C^n(\mathbb{R})$. Hence, $f \notin \mathfrak{W}_n$, so the first two properties in (5.31) hold. Note that $g(x) = (x-i)^{-1} \in \mathfrak{W}_n$ but $g \notin \mathfrak{H}_n$. Therefore, the third property in (5.31) holds.

Below we will also use the notations $u(\lambda) := (\lambda - i)$ and $u^k(\lambda) = (u(\lambda))^k$, $k \in \mathbb{Z}$, $\lambda \in \mathbb{R}$.

Lemma 5.4.4. *For every $f \in \mathfrak{H}_n$,*

$$f^{(k)}u^{k+1} \in C_0(\mathbb{R}), \quad k = 0, \dots, n-1. \tag{5.32}$$

Proof. By the definition of the sets $\mathfrak{H}_n$,

$$f^{(j)}u^j \in L^1(\mathbb{R}), \quad j = 0, 1, \ldots, n.$$

Let $k \in \{0, 1, \ldots, n-1\}$ and $g = f^{(k)}u^{k+1}$. Then, $g' = f^{(k+1)}u^{k+1} + (k+1)f^{(k)}u^k \in L^1(\mathbb{R})$, ensuring that both $\lim_{x\to\infty} g(x)$ and $\lim_{x\to-\infty} g(x)$ exist. Suppose that $\lim_{x\to\infty} g(x) \neq 0$. Then there exist $L, c > 0$ such that for all $x \geq L$ we have $|g(x)| \geq c$, and hence,

$$c\int_L^\infty |u^{-1}(x)|\,dx \leq \int_L^\infty |f^{(k)}(x)u^k(x)|\,dx < \infty,$$

contradicting the definition of u. Therefore, $\lim_{x\to\infty} g(x) = 0$ and, similarly, $\lim_{x\to-\infty} g(x) = 0$. Thus (5.32) holds. □

Lemma 5.4.5. *Let $f \in \mathfrak{H}_n$. Then, $\widehat{f^{(k)}u^l} \in L^1(\mathbb{R})$ for $0 \leq l \leq k \leq n-1$.*

Proof. For $k = l$, the result follows from the definition of $\mathfrak{H}_n$.

Let $l < k$. Since $u^{-k}, u^{-k-1} \in L^2(\mathbb{R})$, we obtain $\widehat{u^{-k}} \in L^1(\mathbb{R})$ for all $k \in \mathbb{N}$ (see, e.g., [**?** , Lemma 7]). By the convolution theorem,

$$\widehat{f^{(k)}u^l} = \left(\widehat{f^{(k)}u^k u^{l-k}}\right) = \widehat{f^{(k)}u^k} * \widehat{u^{l-k}}.$$

Since $L^1(\mathbb{R})$ is closed under the convolution product, $\widehat{f^{(k)}u^l} \in L^1(\mathbb{R})$. □

Lemma 5.4.6. *Let $n \in \mathbb{N}$. Let H_0 be a self-adjoint operator in $\mathcal{H}t$ and let V be a bounded self-adjoint operator on $\mathcal{H}$. Let $H_t = H_0 + tV$, $t \in \mathbb{R}$, and $\tilde{V} = V(H_0 - iI)^{-1}$. Then*

$$\begin{aligned}
&T^{H_t,H_0,\ldots,H_0}_{f^{[n-1]}}(V,\ldots,V) = (-1)^{n-1}f(H_t)\,\tilde{V}^{n-1}\\
&+\sum_{p=1}^{n-1}\sum_{\substack{j_1,\ldots,j_p\geq 1, j_{p+1}\geq 0\\ j_1+\cdots+j_{p+1}=n-1}}(-1)^{n-p-1}\Big(T^{H_t,H_0,\ldots,H_0}_{(fu^{p+1})^{[p]}}(\tilde{V}^{j_1},\ldots,\tilde{V}^{j_p}(H_0-iI)^{-1})\tilde{V}^{j_{p+1}}\\
&\qquad - T^{H_t,H_0,\ldots,H_0}_{(fu^p)^{[p-1]}}(\tilde{V}^{j_1},\ldots,\tilde{V}^{j_{p-1}})\tilde{V}^{j_p}(H_0-iI)^{-1}\tilde{V}^{j_{p+1}}\Big)
\end{aligned}\tag{5.33}$$

for all $f \in \mathfrak{H}_n$.

Proof. The identity (5.33) is trivial in the case $n = 1$.

Let $n \geq 2$. Since $u^{[1]} = 1_{\mathbb{R}^2}$ and $u^{[p]} = 0$ for all $p \geq 2$, the Leibniz rule for divided differences gives

$$(fu)^{[n-1]}(\lambda_0,\ldots,\lambda_{n-1}) = f^{[n-1]}(\lambda_0,\ldots,\lambda_{n-1})u(\lambda_{n-1}) + f^{[n-2]}(\lambda_0,\ldots,\lambda_{n-2}).$$

If we swap λ_{n-1} with λ_j (for any $j \in \{0,\dots,n-1\}$), and rearrange using symmetry of the divided difference, we obtain

$$f^{[n-1]}(\lambda_0,\dots,\lambda_{n-1}) = (fu)^{[n-1]}(\lambda_0,\dots,\lambda_{n-1})u^{-1}(\lambda_j) - f^{[n-2]}(\lambda_0,\dots,\lambda_{j-1},\lambda_{j+1},\dots,\lambda_{n-1})u^{-1}(\lambda_j). \tag{5.34}$$

Applying (5.34) repeatedly, we obtain

$$f^{[n-1]}(\lambda_0,\dots,\lambda_{n-1}) = \sum_{p=0}^{n-1} \sum_{0<j_1<\dots<j_p\le n-1} (-1)^{n-1-p}(fu^p)^{[p]}(\lambda_0,\lambda_{j_1},\dots,\lambda_{j_p})u^{-1}(\lambda_1)\cdots u^{-1}(\lambda_{n-1}). \tag{5.35}$$

By Lemma 5.4.5, $\widehat{f^{(n-1)}}$, $\widehat{(fu^p)^{(p)}} \in L^1(\mathbb{R})$ for $0 \le p \le n-1$. Therefore, applying [52, Lemmas 3.5, 5.1, 5.2] yields

$$T^{H_t,H_0,\dots,H_0}_{f^{[n-1]}}(V,\dots,V) = (-1)^{n-1} f(H_t)\tilde{V}^{n-1} + \sum_{p=1}^{n-1} \sum_{\substack{j_1,\dots,j_p\ge 1, j_{p+1}\ge 0\\ j_1+\dots+j_{p+1}=n-1}} (-1)^{n-1-p}\, T^{H_t,H_0,H_0,\dots,H_0}_{(fu^p)^{[p]}}(\tilde{V}^{j_1},\dots,\tilde{V}^{j_p})\,\tilde{V}^{j_{p+1}}. \tag{5.36}$$

By Lemma 5.4.5 $\widehat{(fu^p)^{(p)}}, \widehat{(fu^{p+1})^{(p)}}$, and $\widehat{(fu^p)^{(p-1)}} \in L^1(\mathbb{R})$ for $1 \le p \le n-1$. Therefore, applying [71, Theorem 3.10(i)] to (5.36) yields (5.33). □

Theorem 5.4.7. *Let $n \in \mathbb{N}$, let H_0 be a self-adjoint operator in $\mathcal{H}$ such that $(H_0 - iI)^{-1} \in \mathcal{B}_n(\mathcal{H})$, and let V be a bounded self-adjoint operator on $\mathcal{H}$. Then, there exists $K_n > 0$ (depending only on n) and a real-valued function η_n such that*

$$|\eta_n(x)| \le K_n\,(2+\|V\|)\,\|V\|^{n-1}\,\|(H_0-iI)^{-1}\|_n^n\,(1+|x|)^n, \quad x \in \mathbb{R}, \tag{5.37}$$

and

$$\mathrm{Tr}(\mathcal{R}_{H_0,f,n}(V)) = \int_{\mathbb{R}} f^{(n)}(x)\eta_n(x)\,dx \tag{5.38}$$

for every $f \in \mathfrak{H}_n \cup \mathfrak{W}_n$. The locally integrable function η_n is determined by (5.38) uniquely up to a polynomial summand of degree at most $n-1$.

Proof. The result for $f \in \mathfrak{W}_n$ is established in [71, Theorem 4.1]. Therefore, there exists a real-valued function $\eta_{\mathfrak{W}_n}$, unique up to a polynomial summand of degree at most $n-1$, satisfying (5.38) for all $f \in \mathfrak{W}_n$.

Now we assume that $f \in \mathfrak{H}_n$. If $n = 1$, then

$$\begin{aligned}|\mathrm{Tr}(\mathcal{R}_{H_0,f,n}(V))| &= |\mathrm{Tr}(f(H_0+V) - f(H_0))| \\ &= |\mathrm{Tr}((fu)(H_0+V)(H_0+V-iI)^{-1} - (fu)(H_0)(H_0-iI)^{-1})| \\ &\le \|fu\|_\infty \,(2+\|V\|)\, \|(H_0-iI)^{-1}\|_1. \end{aligned} \tag{5.39}$$

Let $n \ge 2$. By [71, Theorem 3.13],

$$\begin{aligned}\mathcal{R}_{H_0,f,n}(V) =& \mathcal{R}_{H_0,f,n-1}(V) - \frac{1}{(n-1)!}\frac{d^{n-1}}{ds^{n-1}} f(H_0+sV)\big|_{s=0} \\ =& T^{H_0+V,H_0,\dots,H_0}_{f^{[n-1]}}(V,\dots,V) - T^{H_0,\dots,H_0}_{f^{[n-1]}}(V,\dots,V).\end{aligned} \tag{5.40}$$

Let $H_t = H_0 + tV$, $t \in \mathbb{R}$, and $\tilde{V} = V(H_0 - iI)^{-1}$. By Lemma 5.4.6 applied to (5.40),

$$\begin{aligned}&\mathcal{R}_{H_0,f,n}(V) \qquad (5.41)\\ &= (-1)^{n-1} T^{H_0+V,H_0}_{f^{[1]}}(V)\tilde{V}^{n-1} + \sum_{p=1}^{n-1} \sum_{\substack{j_1,\dots,j_p \ge 1, j_{p+1}\ge 0 \\ j_1+\dots+j_{p+1}=n-1}} (-1)^{n-p-1} \\ &\times \Big[\Big(T^{H_0+V,H_0,\dots,H_0}_{(fu^{p+1})^{[p]}}(\tilde{V}^{j_1},\dots,\tilde{V}^{j_p}(H_0-iI)^{-1}) - T^{H_0,H_0,\dots,H_0}_{(fu^{p+1})^{[p]}}(\tilde{V}^{j_1},\dots,\tilde{V}^{j_p}(H_0-iI)^{-1})\Big)\tilde{V}^{j_{p+1}} \\ &\quad - \Big(T^{H_0+V,H_0,\dots,H_0}_{(fu^p)^{[p-1]}}(\tilde{V}^{j_1},\dots,\tilde{V}^{j_{p-1}}) - T^{H_0,H_0,\dots,H_0}_{(fu^p)^{[p-1]}}(\tilde{V}^{j_1},\dots,\tilde{V}^{j_{p-1}})\Big)\tilde{V}^{j_p}(H_0-iI)^{-1}\tilde{V}^{j_{p+1}}\Big].\end{aligned}$$

By Lemma 5.4.5, $\widehat{f}$, $\widehat{f'}$, $\widehat{(fu)'} \in L^1(\mathbb{R})$. Applying [71, Theorem 3.10(i)] yields

$$T^{H_0+V,H_0}_{f^{[1]}}(V) = T^{H_0+V,H_0}_{(fu)^{[1]}}(\tilde{V}) - f(H_0+V)\tilde{V}. \tag{5.42}$$

Combining (5.41), (5.42), Theorems 5.2.4 and 5.2.5, and applying Hölder's inequality yields

$$\begin{aligned}&|\mathrm{Tr}(\mathcal{R}_{H_0,f,n}(V))| \\ &\le \Big[(\|f\|_\infty + \|(fu)'\|_\infty)\,\|V\|^n + \sum_{p=1}^{n-1} d_{p,n}\,(\|(fu^{p+1})^{(p)}\|_\infty + \|(fu^p)^{(p)}\|_\infty)\,\|V\|^{n-1}\Big]\|(H_0-iI)^{-1}\|_n^n \\ &\le C_n\Big(\sum_{p=1}^{n-1}\|(fu^{p+1})^{(p)}\|_\infty + \sum_{p=0}^{n-1}\|(fu^p)^{(p)}\|_\infty\Big)(1+\|V\|)\|V\|^{n-1}\|(H_0-iI)^{-1}\|_n^n,\end{aligned} \tag{5.43}$$

where C_n is some constant depending only on n. Note that by Lemma 5.4.4, $f^{(k)}u^{k+1} \in C_0(\mathbb{R})$, $k = 0,\dots,n-1$. Arguing similarly to the proof of the existence of the spectral shift function in [71, Proposition 4.2] (that is, by Riesz-Markov representation theorem on each term of (5.41), and then performing integration by parts) we obtain from (5.39) and (5.43) that for each $n \in \mathbb{N}$,

$$\mathrm{Tr}\left(\mathcal{R}_{H_0,f,n}(V)\right) = \int_{\mathbb{R}} f^{(n)}(x)\acute{\eta}_n(x)dx, \tag{5.44}$$

where $\acute{\eta}_n$ is a continuous function on $\mathbb{R}$ such that

$$|\acute{\eta}_n(x)| \leq D_n\left(2 + \|V\|\right)\|V\|^{n-1}\|(H_0 - iI)^{-1}\|_n^n(1 + |x|)^n, \quad x \in \mathbb{R}, \tag{5.45}$$

where D_n is some constant depending only on n. We define

$$\eta_{\mathfrak{H}_n} := \mathrm{Re}\left(\acute{\eta}_n\right).$$

Then it is clear that $\eta_{\mathfrak{H}_n}$ satisfies (5.45) as $|\eta_{\mathfrak{H}_n}| \leq |\acute{\eta}_n|$.

Since the left-hand side of (5.44) is real-valued whenever f is real-valued, we obtain that $\eta_{\mathfrak{H}_n}$ satisfies (5.38) for real-valued $f \in \mathfrak{H}_n$ and, consequently, for all $f \in \mathfrak{H}_n$. The uniqueness of $\eta_{\mathfrak{H}_n}$ satisfying (5.38) up to a polynomial summand of order at most $n-1$ can be established completely analogously to the uniqueness of the function $\eta_{a,b,n,\epsilon,H_0,V}$ established in Theorem 5.3.1. Since both $\eta_{\mathfrak{H}_n}$ and $\eta_{\mathfrak{W}_n}$ satisfy (5.38) for all $f \in C_c^\infty(\mathbb{R})$, by using properties of distributions as in the proof of Theorem 5.3.1, we conclude that $\eta_{\mathfrak{H}_n}$ and $\eta_{\mathfrak{W}_n}$ differ by a polynomial of degree at most $n-1$. Let $\eta_{\mathfrak{H}_n} - \eta_{\mathfrak{W}_n} = Q_n$, where Q_n is a polynomial of degree at most $n-1$. By the property (ii) of Definition 5.4.1, $\int_{\mathbb{R}} f^{(n)}(x)Q_n(x)dx = 0$ for each $f \in \mathfrak{W}_n$. Therefore,

$$\int_{\mathbb{R}} f^{(n)}(x)\eta_{\mathfrak{W}_n}dx = \int_{\mathbb{R}} f^{(n)}(x)(\eta_{\mathfrak{H}_n} - Q_n)dx = \int_{\mathbb{R}} f^{(n)}(x)\eta_{\mathfrak{H}_n}dx,$$

for each $f \in \mathfrak{W}_n$. Hence $\eta_n := \eta_{\mathfrak{H}_n}$ satisfies (5.37) and (5.38) for all $f \in \mathfrak{H}_n \cup \mathfrak{W}_n$. □

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