New York Journal of Mathematics
New York J. Math. **32** (2026) 436–460.

Singular traces and perturbation formulae for tuples of commuting unitaries

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ABSTRACT. We derive a natural generalization of the Krein and Neidhardt trace formulas for tuples of commuting unitaries via a multiplicative path, allowing perturbations to be in a family of Lorentz ideals of bounded linear operators.

CONTENTS

1. Introduction

The Taylor approximation is a fundamental tool in classical function theory, and its operator-theoretic generalization is also a well-known and widely used tool in perturbation theory. One way to study a noncommutative Taylor approximation is by analyzing its properties through traces, an approach known as the trace formula. It was discovered by Lifshitz [20] in a special case and by Krein [18] in a general case.

Let $\mathcal{H}$ denote a complex separable Hilbert space, $\mathcal{B}(\mathcal{H})$ the algebra of all bounded linear operators on $\mathcal{H}$, and $\mathcal{S}^n(\mathcal{H})$ the n-th Schatten-von Neumann ideal of compact operators on $\mathcal{H}$ (see [16] for a detailed discussion on their properties). Initial trace formulas were derived for trace class perturbations $\mathcal{S}^1(\mathcal{H})$ of either a self-adjoint operator H_0 or a unitary operator U_0, and allowed to efficiently compute the perturbed operator functions $f(H_0+V)$ and $f(e^{iA}U_0)$

Received April 9, 2025.
2010 *Mathematics Subject Classification.* 47A55, 47B10, 47A13.
Key words and phrases. Krein trace formula, Neidhardt trace formula, Lorentz ideal, singular trace.

ISSN 1076-9803/2026

in terms of the initial data, namely:

$$\operatorname{Tr}\{f(H_0+V)-f(H_0)\}=\int_{\mathbb{R}} f'(\lambda)d\nu(\lambda) \tag{1.1}$$

and

$$\operatorname{Tr}\left\{f(e^{iA}U_0)-f(U_0)\right\}=\int_{\mathbb{T}} f'(z)\,d\mu(z). \tag{1.2}$$

Here, Tr denotes the standard trace on $\mathcal{S}^1(\mathcal{H})$. The relations (1.1) and (1.2) are known as the *Krein trace formulas* for pairs of self-adjoint [18] and unitary operators [19], respectively, and the measures ν and μ are called spectral shift measures (in short, SSM). We refer to [23] and [1] for the description of the maximal class of functions for which (1.1) and (1.2) hold, respectively.

The extensions of (1.1) and (1.2) to Hilbert–Schmidt perturbations $\mathcal{S}^2(\mathcal{H})$ are due to Koplienko [17] and Neidhardt [22], respectively. Let U and U_0 be two unitary operators on $\mathcal{H}$ such that $U-U_0\in\mathcal{S}^2(\mathcal{H})$. Then $U=e^{iA}U_0$, where $A=A^*\in\mathcal{S}^2(\mathcal{H})$. Denote $U(s)=e^{isA}U_0$, where $s\in\mathbb{R}$. Then, there exist measures μ_1 and μ_2 on $\mathbb{T}$ such that

$$\operatorname{Tr}\left\{f(e^{iA}U_0)-f(U_0)-\frac{d}{ds}\bigg|_{s=0} f(U(s))\right\}=\sum_{k=1}^{2}\int_{\mathbb{T}} f^{(k)}(z)\,d\mu_k(z), \tag{1.3}$$

whenever f'' has absolutely convergent Fourier series. Neidhardt's elegant result (1.3) is known as the *Neidhardt trace formula*. An interested reader can see [24] and [25] for the recent developments on higher order trace formulas with perturbation operators from the Schatten-von Neumann ideal. For more on the history of the subject, we refer the reader to [28] and the references cited therein.

We note that all the spectral shift measures in (1.1)–(1.3) are absolutely continuous with respect to the Lebesgue measure. We remind the reader that spectral shift measures are known for their applications in spectral flow [3] and scattering theory [4], just to name a few. In addition, the first order SSM has appeared in inverse problems for one-dimensional Schrödinger, Dirac, and Jacobi operators [9].

Taylor-like approximations have been fairly well investigated in the single-variable case. Now it is worth exploring its several variable generalizations, which is a common occurrence in the classical case. Although several recent works, such as [29], [2] and [6] have studied the multivariable counterpart of one variable trace formulas, it remains largely unexplored. Specifically, [6] establishes a multivariate analog of (1.1) for tuples of commuting self-adjoint operators. In contrast, [29] focuses on tuples of commuting contractions that admit a dilation to tuples of commuting normal contractions. Note that Krein's trace formula (1.1) does not hold for functions of pairs of noncommuting self-adjoint operators (see [2]).

It is well known that, in the one variable setting for contractions, higher order trace formulas take different forms depending on whether the differentiation is performed along the linear path $t \mapsto T_0 + t(T - T_0)$ or the multiplicative path $t \mapsto e^{itA}T_0$, where $T - T_0, A = A^* \in \mathcal{B}(\mathcal{H})$. Both approaches have been extensively studied in the literature (see, e.g., [7, 25, 26]) and have found significant applications.

We want to mention that there has been significant progress in deriving trace formulas for self-adjoint operators with non-compact perturbations in the single variable case, where these results find applications in the study of Dirac and Schrödinger operators (see, e.g., [8, 22, 30, 33]). Trace formulas for unitary operators, especially those developed via the multiplicative path, have played a crucial role in these developments (see [22, 30]). This serves as the primary motivation for establishing trace formulas for functions of n-tuple of commuting unitaries via the multiplicative path, which are missing in [29] (where only the linear path is considered). A further advantage of the multiplicative path approach is that it allows us to establish trace formulas for a larger class of functions, including non-analytic functions (see Theorems 1.1 and 1.2). Note that the trace formulas in [29] are restricted only to analytic functions.

The perturbation formulas (1.1)-(1.3) have been extended to include more general perturbations. In [15, Theorem 3.13], (1.2) has been studied in the context of general symmetrically normed ideals of semifinite von Neumann algebras, which include the trace class ideal and the Lorentz ideal (see Section 2.1).

Lorentz ideals with singular traces (traces that vanish on finite rank operators) are closely related to important objects of perturbation theory - see, for example, [10], where Connes used singular traces as a cornerstone of his work in noncommutative geometry and calculus. The development of perturbation formulas for singular traces has opened up new possibilities for applications; for instance, see [27]. These remarkable connections inspired us to establish multivariable counterparts of (1.2) and (1.3) with perturbations from Lorentz ideals. Moreover the singularity of the trace plays a crucial role (as we can see in the proofs of Theorems 1.1 and 1.2) to derive our main results under the assumption of only the commutativity of the initial operator tuples. This also highlights an interesting behavior of singular traces. We will further comment at the end of the paper on possible extensions of our main results to the case of perturbations from the trace class and Hilbert–Schmidt ideals.

1.1. Summary of main results.

Let $\mathcal{U}(\mathcal{H})$ denote the collection of all unitaries on $\mathcal{H}$. Let $\psi : (0, \infty) \to (0, \infty)$ be a concave function such that

$$\lim_{t\to\infty} \psi(t) = \infty.$$

Then the Lorentz ideal associated to ψ is denoted by $\mathcal{M}_\psi$ and consists of all compact operators A such that

$$\sup_{n\geq 0} \frac{1}{\psi(1+n)} \sum_{k=0}^{n} \lambda_k(A) < \infty,$$

where $\{\lambda_k(A)\}_{k=0}^{\infty}$ denotes the singular value sequence of A. Throughout the article, we consider perturbations in the Lorentz ideal $\mathcal{M}_\psi$ and in its root ideal $\mathcal{M}_\psi^{1/2} = \{A \in \mathcal{B}(\mathcal{H}) : |A|^2 \in \mathcal{M}_\psi\}$. For more details on the Lorentz ideal, we refer the reader to Section 2.1.

Let τ_ψ be a bounded singular trace on $\mathcal{M}_\psi$. Assume that the function ψ satisfies

$$\psi(t) \leq Ct^{\varepsilon}, \quad t \geq 1 \tag{1.4}$$

for some constant $C > 0$ and $0 < \varepsilon < 1$.

Let $m, n \in \mathbb{N}$ with $n \geq 2$. Denote by Com_n the set of all n-tuple of pairwise commuting elements in $\mathcal{B}(\mathcal{H})$. Consider a tuple of unitary operators $\mathbf{U}_n := (U_1, \dots, U_n)$. Define

$$\mathbf{U}_n(t) := (e^{itA_1}U_1, \dots, e^{itA_n}U_n),$$

where $t \in \mathbb{R}$ and $\mathbf{A}_n := (A_1, \dots, A_n)$ is a tuple of bounded self-adjoint operators. For an n-tuple of unitary operators $\mathbf{U}_n$ and a perturbed n-tuple $\mathbf{U}_n(1)$, and for a sufficiently smooth function $f : \mathbb{T}^n \to \mathbb{C}$, the m-th order Taylor remainder is denoted by $\mathcal{R}_m(f, \mathbf{U}_n, \mathbf{A}_n)$ and is defined by

$$\mathcal{R}_m(f, \mathbf{U}_n, \mathbf{A}_n) := f(\mathbf{U}_n(1)) - f(\mathbf{U}_n) - \sum_{k=1}^{m-1} \frac{1}{k!} \frac{d^k}{ds^k}\bigg|_{s=0} f(\mathbf{U}_n(s)). \tag{1.5}$$

Denote by $\mathcal{F}_m(\mathbb{T}^n)$ the collection of all functions $f \in C^m(\mathbb{T}^n)$ for which $\mathcal{D}^k f$ has an absolutely convergent Fourier series for each $0 \leq k \leq m$, where

$$\mathcal{D}^k f := \frac{\partial^k f}{\partial z_1^{\alpha_1} \cdots \partial z_n^{\alpha_n}},$$

with $\alpha_1, \dots, \alpha_n \geq 0$ and $\alpha_1 + \cdots + \alpha_n = k$.

With this background, we now list the main contributions of this article.

Theorem 1.1. *Let $\mathcal{M}_\psi$ be the Lorentz ideal and suppose the function ψ satisfies (1.4) for some $0 < \varepsilon < 1/2$. Let τ_ψ be a bounded singular trace on it. Consider two n-tuple of operators $\boldsymbol{U}_n$ and $\boldsymbol{A}_n$ such that $U_j \in \mathcal{U}(\mathcal{H})$ and $A_j = A_j^* \in \mathcal{M}_\psi$ for $j = 1, \dots, n$. Suppose that $\boldsymbol{U}_n \in \mathrm{Com}_n$. Then, there exist measures $\mu_1, \dots, \mu_n$ on $\mathbb{T}^n$ such that*

$$\|\mu_j\| \leq \|\tau_\psi\|_{\mathcal{M}_\psi^*} \|A_j\|_{\mathcal{M}_\psi}, \ 1 \leq j \leq n$$

and

$$\tau_\psi\{\mathcal{R}_1(f, \boldsymbol{U}_n, \boldsymbol{A}_n)\} = \sum_{j=1}^{n} \int_{\mathbb{T}^n} \frac{\partial f}{\partial z_j}(z_1, \dots, z_n)\, d\mu_j(z_1, \dots, z_n),$$

for every $f \in \mathcal{F}_2(\mathbb{T}^n)$.

In Theorem 1.1 of this paper, we relax the assumptions on operators made in [29, Proposition 3.12] (where $\mathbf{U}_n, \mathbf{U}_n(1) \in \mathrm{Com}_n$ were considered), and enlarge the class of admissible functions to include non-analytic functions.

Theorem 1.2. *Let $\mathcal{M}_\psi$ be the Lorentz ideal and suppose the function ψ satisfies (1.4) for some $0 < \varepsilon < 1/3$. Let τ_ψ be a bounded singular trace on it. Consider two n-tuple of operators $\boldsymbol{U}_n$ and $\boldsymbol{A}_n$ such that $U_j \in \mathcal{U}(\mathcal{H})$ and $A_j = A_j^* \in \mathcal{M}_\psi^{1/2}$ for $j = 1, \ldots, n$. Suppose that $\boldsymbol{U}_n \in \mathrm{Com}_n$. Then, there exist finite measures μ_{ij}, ν_j for $1 \leq i \leq j \leq n$ on $\mathbb{T}^n$ such that*

$$\tau_\psi\{\mathcal{R}_2(f, \boldsymbol{U}_n, \boldsymbol{A}_n)\} = \sum_{1\leq i\leq j\leq n} \int_{\mathbb{T}^n} \frac{\partial^2 f}{\partial z_i \partial z_j}(z_1, \ldots, z_n)\, d\mu_{ij}(z_1, \ldots, z_n) + \sum_{1\leq j\leq n} \int_{\mathbb{T}^n} \frac{\partial f}{\partial z_j}(z_1, \ldots, z_n)\, d\nu_j(z_1, \ldots, z_n),$$

for every $f \in \mathcal{F}_3(\mathbb{T}^n)$.

We refer the reader to Remark 5.2 for the total variation of the measures obtained in Theorem 1.2.

It is noteworthy to mention that the results in [29] are established only for positive traces (see [29, Hypotheses 3.3]). In contrast, our main results are derived for traces that are not necessarily positive. Furthermore, the techniques developed in this article allow us to establish our results under the weaker assumption that $\mathbf{U}_n \in \mathrm{Com}_n$ only. This weaker assumption is sufficiently general for applications.

Finally, a few words about this paper's methodology. Both the proofs of Theorem 1.1 and Theorem 1.2 rely on the singularity of the trace τ_ψ. Our approach is partly based on the methods considered in [29] and [15]. A key element of the proof of Theorem 1.2 is the estimate (5.1) (see also Theorem 5.1), which is based on the estimates of the divided differences (see Lemma 3.4). Additionally, we have utilized the Riesz-Markov representation theorem and the classical Hahn-Banach theorem.

Now, we discuss the layout of this paper. Apart from the Introduction, this article has four sections. Section 2 contains notations and preliminaries on Lorentz ideal. In Section 3, we derive the essential estimates for the first and second order divided differences. Section 4 deals with the first order perturbation formula, while Section 5 establishes the second order perturbation formula for tuples of commuting unitaries.

2. Notations and preliminaries

Notations: We use the following standard notations: $\mathbb{N}, \mathbb{Z}_+, \mathbb{Z}, \mathbb{R}$, and $\mathbb{C}$ represent the sets of natural numbers, non-negative integers, integers, real numbers, and complex numbers, respectively. Throughout the paper, n will denote a natural number with $n \geq 2$. The set $\mathbb{Z}^n$ consists of all n-tuple of integers. We also represent $k \in \mathbb{Z}^n$ by the tuple $(k_1, \ldots, k_n)$, where each $k_i \in \mathbb{Z}$. Additionally, $\mathbb{T}$ stands for the unit circle in $\mathbb{C}$, and $\mathbb{T}^n$ represents the n-dimensional torus in $\mathbb{C}^n$.

1. $\mathcal{U}(\mathcal{H})$ denotes the collection of all unitaries on $\mathcal{H}$.

2. Denote by Com_n the set of all n-tuple of pairwise commuting elements in $\mathcal{B}(\mathcal{H})$.
3. The n-tuple of bounded operators $A_1, \dots, A_n$ is denoted by

$$\mathbf{A}_n = (A_1, \dots, A_n),$$

and

$$\mathbf{U}_n(t) = (U_1(t), \dots, U_n(t))$$

denotes the n-tuple of operators with each $U_j : \mathbb{R} \to \mathcal{U}(\mathcal{H})$. For notational simplicity, we define for $k_1, \dots, k_n \in \mathbb{Z}$:

$$T_{k_i,\dots,k_j}(t) = \prod_{l=i}^{j} U_l(t)^{k_l}, \text{ for } 1 \le i \le j \le n. \tag{2.1}$$

Definition 2.1. A trace $\tau_{\mathcal{J}}$ on a two-sided ideal $\mathcal{J}$ of $\mathcal{B}(\mathcal{H})$ is a unitarily invariant linear functional, that is,

$$\tau_{\mathcal{J}}(UAU^*) = \tau_{\mathcal{J}}(A)$$

for all $A \in \mathcal{J}$ and all unitary operators $U \in \mathcal{B}(\mathcal{H})$.

We say the trace $\tau_{\mathcal{J}}$ is
- positive if $A \in \mathcal{J}$, $A \ge 0$ implies $\tau_{\mathcal{J}}(A) \ge 0$;
- bounded on $\mathcal{J}$ if there exists a constant $M > 0$ such that

$$|\,\tau_{\mathcal{J}}(A)| \le M\|A\|_{\mathcal{J}}, \text{ for all } A \in \mathcal{J}.$$

The infimum of such M equals $\|\,\tau_{\mathcal{J}}\,\|_{\mathcal{J}^*}$;
- singular if it vanishes on finite rank operators.

Note that we do not require a trace to be positive.

2.1. Lorentz ideal. Let $\psi : (0,\infty) \to (0,\infty)$ be a concave function such that $\lim_{t\to\infty} \psi(t) = \infty$. Then the Lorentz ideals are defined by

$$\mathcal{M}_\psi = \Big\{A \in \mathcal{B}(\mathcal{H}) \text{ is compact} : \|A\|_{\mathcal{M}_\psi} := \sup_{n\ge 0} \frac{1}{\psi(1+n)} \sum_{k=0}^{n} \lambda_k(A) < \infty\Big\},$$

where $\{\lambda_k(A)\}_{k=0}^{\infty}$ is a singular value sequence of A. More information about singular values can be found in [16, Chapter II]. Moreover, the norm $\|\cdot\|_{\mathcal{M}_\psi}$ makes $\mathcal{M}_\psi$ into a symmetrically normed ideal (see [21, Definition 1.2.12]). In particular, we have the following property: if $B \in \mathcal{M}_\psi$ and $A, C \in \mathcal{B}(\mathcal{H})$, then $AB, BC \in \mathcal{M}_\psi$ and $\|ABC\|_{\mathcal{M}_\psi} \le \|A\|\|B\|_{\mathcal{M}_\psi}\|C\|$. This follows from properties of the singular value sequence [16, p. 27].

In 1966, J. Dixmier [13] discovered traces that vanish on finite rank operators. In fact, he considered the following functional

$$\mathrm{Tr}_\omega(A) = \omega\Big(\Big\{\frac{1}{\psi(1+n)} \sum_{k=0}^{n} \lambda_k(A)\Big\}_{n\ge 0}\Big), \quad 0 \le A \in \mathcal{M}_\psi, \tag{2.2}$$

where ω is a dilation invariant state on the algebra of all bounded sequences ℓ_∞, that is, invariant with respect to the dilation semigroup $\sigma_n : \ell_\infty \to \ell_\infty$, $n \geq 1$, defined by setting

$$\sigma_n(a_0, a_1, \ldots) = (\underbrace{a_0, \ldots, a_0}_{n \text{ times}}, \underbrace{a_1, \ldots, a_1}_{n \text{ times}}, \ldots).$$

Note that Tr_ω extends by linearity to the whole ideal $\mathcal{M}_\psi$. Nowadays, functionals of the form (2.2) are termed Dixmier traces. In [14, Theorem 3.4], the authors have shown that $\mathcal{M}_\psi$ admits non-trivial Dixmier traces if and only if

$$\liminf_{t\to\infty} \frac{\psi(2t)}{\psi(t)} = 1.$$

Later on, it became clear that there are a plethora of singular traces other than Dixmier traces.

For every $\alpha > 0$, we have the root ideal

$$\mathcal{M}_\psi^\alpha = \{A \in \mathcal{B}(\mathcal{H}) \text{ is compact} : |A|^{1/\alpha} \in \mathcal{M}_\psi\}.$$

Let τ_ψ be a bounded singular trace on $\mathcal{M}_\psi$. If for some $0 < \varepsilon < 1$ there exists a constant $C > 0$ such that

$$\psi(t) \leq Ct^\varepsilon, \quad t \geq 1, \tag{2.3}$$

then according to [6, Proposition 2.3] we have

$$\tau_\psi(\mathcal{M}_\psi^\alpha) = \{0\} \quad \text{for every} \quad \alpha > \frac{1}{1-\varepsilon}. \tag{2.4}$$

There are many Lorentz ideals satisfying (2.3). In particular, these conditions are met by the Lorentz ideal with $\psi(t) = \log(t)$. We will take advantage of property (2.4) in the proof of our main results.

We also consider perturbations in the root ideal $\mathcal{M}_\psi^{1/2}$. Note that, $\mathcal{M}_\psi^{1/2}$ is a normed ideal with the norm $\|A\|_{\mathcal{M}_\psi^{1/2}} = \||A|^2\|_{\mathcal{M}_\psi}^{1/2}$ (see [15, Proposition 2.5]). For the second order perturbation formula we need the following Hölder-like inequality from [15, Proposition 2.5]:

$$\|AB\|_{\mathcal{M}_\psi} \leq \|A\|_{\mathcal{M}_\psi^{1/2}} \|B\|_{\mathcal{M}_\psi^{1/2}} \quad \text{for all} \quad A, B \in \mathcal{M}_\psi^{1/2}. \tag{2.5}$$

From now on, we will use the notation $\mathcal{M}_\psi$ and τ_ψ to refer the Lorentz ideal and a bounded singular trace on it, respectively.

2.2. Function spaces. Let $m \in \mathbb{N}$. Let $C^m(\mathbb{T}^n)$ denote the space of all m-times continuously differentiable functions on $\mathbb{T}^n$. For $m = 0$, we use the convention that $C^0(\mathbb{T}^n) = C(\mathbb{T}^n)$, the space of all continuous functions on $\mathbb{T}^n$. Denote

$$\mathcal{F}_m(\mathbb{T}^n) := \Big\{ f \in C^m(\mathbb{T}^n) \mid \mathcal{D}^k f \text{ has absolute convergent Fourier series for } 0 \leq k \leq m \Big\}, \tag{2.6}$$

where $\mathcal{D}^k f := \dfrac{\partial^k f}{\partial z_1^{\alpha_1} \cdots \partial z_n^{\alpha_n}}$, $\alpha_1, \dots, \alpha_n \geq 0$, $\alpha_1 + \cdots + \alpha_n = k$.

Consider the function

$$f(z_1, \dots, z_n) = \sum_{k \in \mathbb{Z}^n} \widehat{f}(k)\, z_1^{k_1} \cdots z_n^{k_n}, \tag{2.7}$$

where $(z_1, \dots, z_n) \in \mathbb{T}^n$ and $\sum_{k \in \mathbb{Z}^n} \left|\widehat{f}(k)\right| < \infty$. We then define the operator function by

$$f(U_1, \dots, U_n) = \sum_{k \in \mathbb{Z}^n} \widehat{f}(k)\, U_1^{k_1} \cdots U_n^{k_n},$$

for a tuple of unitaries $(U_1, \dots, U_n)$, which are not necessarily commuting.

Recall that, for a tuple of commuting unitaries $\mathbf{U}_n$ and given a bounded Borel function f on $\sigma(\mathbf{U}_n)$ (the joint spectrum of the operators $U_1, \dots, U_n$), the operator function $f(\mathbf{U}_n)$ is representable by the integral

$$f(\mathbf{U}_n) = \underbrace{\int \cdots \int}_{\sigma(\mathbf{U}_n)} f(\lambda_1, \dots, \lambda_n)\, dE(\lambda_1, \dots, \lambda_n),$$

where E is the product of the spectral measures E_j of the operators U_j, $1 \leq j \leq n$ [5, Theorem 6.5.1 and Subsection 6.6.2], and it is supported on $\sigma(\mathbf{U}_n)$. By the spectral theorem for an n-tuple of commuting unitaries $\mathbf{U}_n$, it follows that:

$$\|f(\mathbf{U}_n)\| \leq \|f\|_{L^\infty(\mathbb{T}^n)}, \tag{2.8}$$

for $f \in \mathcal{F}_1(\mathbb{T}^n)$.

3. Preparatory results

The aim of this section is to collect some key results from the literature and prove some new results, which we need subsequently. Again, we remind the reader that throughout the paper, n will denote a natural number, and (unless otherwise stated) we always assume that $n \geq 2$.

We begin this section with the following result, which is well-known for trace class ideal (see, e.g., [30, p. 504]). However, this result also holds for Lorentz ideals $\mathcal{M}_\psi$. The proof follows a similar line of arguments as in ([30, p. 504]).

Theorem 3.1. *Let $U, U_0 \in \mathcal{U}(\mathcal{H})$ be such that $U - U_0 \in \mathcal{M}_\psi$ (resp. $\mathcal{M}_\psi^{1/2}$). Then, there exists $A = A^* \in \mathcal{M}_\psi$ (resp. $\mathcal{M}_\psi^{1/2}$) such that $U = e^{iA} U_0$.*

To proceed further, we need the following lemma, which gives the general formula for the n-th derivative of the function $t \in \mathbb{R} \mapsto (e^{itA}U)^p$, for $p \in \mathbb{Z}$.

Note that, the following result is a particular case of [31, Theorem 5.3.4], where the derivative is expressed in terms of multiple operator integrals, which is not useful for our purpose. Instead, we present the following expression, which is particularly useful for our situation.

Lemma 3.2. *Let $p \in \mathbb{Z}$, and define $U(t) = e^{itA}U$ for $t \in \mathbb{R}$, where $A = A^* \in \mathcal{B}(\mathcal{H})$ and $U \in \mathcal{U}(\mathcal{H})$. Then, for all $n \in \mathbb{N}$, the following assertions hold.*

(i) *If $p > 0$, then*

$$\frac{d^n}{ds^n}\bigg|_{s=t}\{U(s)^p\} = i^n \sum_{r=1}^{\min\{n,p\}} \sum_{\substack{l_1,\dots,l_r \geq 1\\ l_1+\cdots+l_r=n}} \frac{n!}{l_1!\cdots l_r!} \times \Bigg[\sum_{\substack{\alpha_0,\dots,\alpha_r\geq 0\\ \alpha_0+\cdots+\alpha_r=p-r}} U(t)^{\alpha_0}\Bigg\{\prod_{j=1}^{r} A^{l_j}U(t)^{\alpha_j+1}\Bigg\}\Bigg]. \tag{3.1}$$

(ii) *If $p < 0$, then*

$$\frac{d^n}{ds^n}\bigg|_{s=t}\{U(s)^p\} = i^n \sum_{r=1}^{n} \sum_{\substack{l_1,\dots,l_r \geq 1\\ l_1+\cdots+l_r=n}} \frac{n!}{l_1!\cdots l_r!} \times \Bigg[\sum_{\substack{\alpha_0,\dots,\alpha_r\geq 0\\ \alpha_0+\cdots+\alpha_r=|p|-1}} U(t)^{-\alpha_0-1}\Bigg\{\prod_{j=1}^{r} (-A^{l_j})U(t)^{-\alpha_j}\Bigg\}\Bigg]. \tag{3.2}$$

The derivatives in (3.1) and (3.2) both exist in operator norm. Moreover, if $A \in \mathcal{M}_\psi$, then for $n \geq 1$, the derivatives exist in the norm $\|\cdot\|_{\mathcal{M}_\psi}$. If $A \in \mathcal{M}_\psi^{1/2}$, they exist in the norm $\|\cdot\|_{\mathcal{M}_\psi^{1/2}}$ for $n = 1$ and in the norm $\|\cdot\|_{\mathcal{M}_\psi}$ for $n \geq 2$.

The following theorem establishes the differentiability of $t \mapsto f(\mathbf{U}_n(t))$ for $f \in \mathcal{F}_m(\mathbb{T}^n)$. By making proper adjustments in the proof of [29, Lemma 3.2], one can obtain the following theorem; hence, the detailed proof is left to the reader.

Theorem 3.3. *Consider $\boldsymbol{U}_n(t) = (e^{itA_1}U_1, \dots, e^{itA_n}U_n)$ for $t \in \mathbb{R}$, where $A_j = A_j^* \in \mathcal{B}(\mathcal{H})$ and $U_j \in \mathcal{U}(\mathcal{H})$ for $j = 1, \dots, n$. Then,*

(i) *for $f \in \mathcal{F}_2(\mathbb{T}^n)$*

$$\frac{d}{ds}\bigg|_{s=t} f(\boldsymbol{U}_n(s)) = \sum_{j=1}^{n} D_j^f(t), \tag{3.3}$$

where

$$D_j^f(t) = \sum_{k\in\mathbb{Z}^n} \hat{f}(k)T_{k_1,\dots,K_{j-1}}(t)\frac{d}{ds}\bigg|_{s=t} U_j(s)^{k_j}T_{k_{j+1},\dots,k_n}(t). \tag{3.4}$$

(ii) *for $f \in \mathcal{F}_3(\mathbb{T}^n)$*

$$\frac{d^2}{ds^2}\bigg|_{s=t} f(\boldsymbol{U}_n(s)) = 2\sum_{1\leq i<j\leq n} D_{i,j}^f(t) + \sum_{1\leq j\leq n} D_{j,j}^f(t), \tag{3.5}$$

where

$$D_{i,j}^{f}(t) = \sum_{k\in\mathbb{Z}^n} \widehat{f}(k) T_{k_1,\dots,k_{i-1}}(t) \frac{d}{ds}\Big|_{s=t} U_i(s)^{k_i} T_{k_{i+1},\dots,k_{j-1}}(t) \times \frac{d}{ds}\Big|_{s=t} U_j(s)^{k_j} T_{k_{j+1},\dots,k_n}(t), \tag{3.6}$$

and

$$D_{j,j}^{f}(t) = \sum_{k\in\mathbb{Z}^n} \widehat{f}(k) T_{k_1,\dots,k_{j-1}}(t) \frac{d^2}{ds^2}\Big|_{s=t} U_j(s)^{k_j} T_{k_{j+1},\dots,k_n}(t). \tag{3.7}$$

The derivatives in (3.3) and (3.5) both exist and are continuous in the operator norm. Additionally, if $A_j \in \mathcal{M}_\psi$, $1 \le j \le n$, then (3.3) exists in the $\|\cdot\|_{\mathcal{M}_\psi}$-norm, and if $A_j \in \mathcal{M}_\psi^{1/2}$, $1 \le j \le n$, then (3.5) exists in the $\|\cdot\|_{\mathcal{M}_\psi}$-norm.

Now, let's delve into one of the key tools, the divided difference. We recall that the zeroth order divided difference of a function $\varphi : \mathbb{T} \to \mathbb{C}$ is simply the function itself, that is, $\varphi[\lambda] = \varphi(\lambda)$. Let $m \in \mathbb{N}$. Consider points $\lambda_0, \lambda_1, \dots, \lambda_m$ in $\mathbb{T}$ and let $\varphi \in C^m(\mathbb{T})$. Then the m-th order divided difference of φ is defined recursively by

$$\varphi[\lambda_0, \dots, \lambda_m] = \lim_{\lambda\to\lambda_m} \frac{\varphi[\lambda_0, \dots, \lambda_{m-2}, \lambda] - \varphi[\lambda_0, \dots, \lambda_{m-2}, \lambda_{m-1}]}{\lambda - \lambda_{m-1}}. \tag{3.8}$$

It is important to note that $\varphi[\lambda_0, \dots, \lambda_m]$ is a symmetric function of the sequence $\{\lambda_0, \dots, \lambda_m\}$. Basic properties of divided difference can be found in, for example, [12, Section 4.7].

Let f be a function on $\mathbb{T}^n$ and $f \in C^m(\mathbb{T}^n)$. We define the m-th order divided difference of f in the i-th coordinate [29] by

$$f(z_1, \dots, z_{i-1}, [\lambda_0, \dots, \lambda_m], z_{i+1}, \dots, z_n) = \varphi_i[\lambda_0, \dots, \lambda_m],$$

where

$$\varphi_i(\lambda) = f(z_1, \dots, z_{i-1}, \lambda, z_{i+1}, \dots, z_n), \tag{3.9}$$

and $z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_n$ are fixed points in $\mathbb{T}$.

Let $z := (z_1, \dots, z_n) \in \mathbb{T}^n$, $\lambda_1, \lambda_2, \mu_1, \mu_2 \in \mathbb{T}$ and $f \in \mathcal{F}_2(\mathbb{T}^n)$ with the representation given by (2.7). Define

$$\mathcal{D}^i_{[\lambda_1,\lambda_2]} f(z) = f(z_1, \dots, z_{i-1}, [\lambda_1, \lambda_2], z_{i+1}, \dots, z_n),$$

and

$$\begin{aligned} &\mathcal{D}^{i,j}_{[\lambda_1,\lambda_2],[\mu_1,\mu_2]} f(z) \\ =&\mathcal{D}^i_{[\lambda_1,\lambda_2]} \cdot \mathcal{D}^j_{[\mu_1,\mu_2]} f(z) \\ =&f\left(z_1, \dots, z_{i-1}, [\lambda_1, \lambda_2], z_{i+1}, \dots, z_{j-1}, [\mu_1, \mu_2], z_{j+1}, \dots, z_n\right). \end{aligned}$$

Note that,

$$\mathcal{D}^i_{[\lambda_1,\lambda_2]} \cdot \mathcal{D}^j_{[\mu_1,\mu_2]} f(z) = \mathcal{D}^j_{[\mu_1,\mu_2]} \cdot \mathcal{D}^i_{[\lambda_1,\lambda_2]} f(z).$$

We need the following estimates for the sup-norm of the divided difference.

Lemma 3.4. *Let* $f \in \mathcal{F}_2(\mathbb{T}^n)$ *and* $z := (z_1, \dots, z_n) \in \mathbb{T}^n$*. Then, the following assertions hold.*

(i) *If* $\lambda_1, \lambda_2, \mu_1, \mu_2 \in \mathbb{T}$ *then*

$$\sup_{\lambda_1,\lambda_2,\mu_1,\mu_2\in\mathbb{T}; z\in\mathbb{T}^n} \left|\mathcal{D}^{i,j}_{[\lambda_1,\lambda_2],[\mu_1,\mu_2]} f(z)\right| \le \left(\frac{\pi}{2}\right)^2 \left\|\frac{\partial^2 f}{\partial z_i \partial z_j}\right\|_\infty . \tag{3.10}$$

(ii) *If* $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{T}$ *then*

$$\sup_{z_1,\dots,z_n,\lambda_1,\lambda_2,\lambda_3\in\mathbb{T}} \left|f(z_1, \dots, z_{j-1}, [\lambda_1, \lambda_2, \lambda_3], z_{j+1}, \dots, z_n)\right| \le \left(\frac{\pi}{2}\right) \left\|\frac{\partial^2 f}{\partial z_j^2}\right\|_\infty . \tag{3.11}$$

Proof. The proof is essentially an argument of Curtiss [11], but for the reader's convenience we present it here.

(i) We first prove (i). The proof is obtained by elementary methods and involves integral representations. Assume $\lambda_1 \neq \lambda_2$ and $\mu_1 \neq \mu_2$. Firstly, we represent the divided difference as an integral over the circular arc

$$\mathcal{D}^j_{[\mu_1,\mu_2]} f(z) = \frac{1}{e^{i\theta_2} - e^{i\theta_1}} \int_{\theta_1}^{\theta_2} \frac{\partial f}{\partial z_j} \left(z_1, \dots, z_{j-1}, e^{it}, z_{j+1}, \dots, z_n\right) ie^{it}\, dt, \tag{3.12}$$

where $\mu_1 = e^{i\theta_1}, \mu_2 = e^{i\theta_2}$, with θ_1 and θ_2 are such that $|\theta_2 - \theta_1| \le \pi$.
Similarly, we obtain

$$\mathcal{D}^{i,j}_{[\lambda_1,\lambda_2],[\mu_1,\mu_2]} f(z) = \frac{-1}{\left(e^{i\theta_2} - e^{i\theta_1}\right)\left(e^{i\theta_4} - e^{i\theta_3}\right)} \int_{\theta_1}^{\theta_2} \int_{\theta_3}^{\theta_4} \Psi_f(z, s, t) ds dt, \tag{3.13}$$

where

$$\Psi_f(z, s, t) := \frac{\partial^2 f}{\partial z_i \partial z_j} \left(z_1, \dots, z_{i-1}, e^{is}, z_{i+1}, \dots, z_{j-1}, e^{it}, z_{j+1}, \dots, z_n\right) e^{i(s+t)},$$

with $\lambda_1 = e^{i\theta_3}, \lambda_2 = e^{i\theta_4}$, and where θ_3 and θ_4 are such that $|\theta_4 - \theta_3| \le \pi$.
On the other hand, by utilizing the inequality:

$$|\sin\theta| \ge |2\theta/\pi|, \quad \text{for } -\frac{\pi}{2} \le \theta \le \frac{\pi}{2},$$

we derive

$$\left|e^{i\theta} - e^{i\zeta}\right| = 2\left|\sin\left(\frac{\theta - \zeta}{2}\right)\right| \ge \frac{2}{\pi}|\theta - \zeta|, \quad \text{for } |\theta - \zeta| \le \pi. \tag{3.14}$$

Finally, combining (3.13) with (3.14) establishes the inequality (3.10). The proof in the general case follows similarly.

(ii) We now prove (ii). Consider

$$\varphi(\xi) = f(z_1, \dots, z_{j-1}, \xi, z_{j+1}, \dots, z_n),$$

where $z_1, \dots, z_{j-1}, z_{j+1}, \dots, z_n$ are fixed points in $\mathbb{T}$. Now, the proof is divided into two cases.

`Case 1:` $\lambda_1, \lambda_2, \lambda_3$ are distinct.

Then, by [11, Theorem 2.1] we have

$$|\varphi[\lambda_1, \lambda_2, \lambda_3]| \leq \left(\frac{\pi}{2}\right) \left\| \frac{\partial^2 f}{\partial z_j^2} \right\|_\infty \quad \text{for all distinct } \lambda_1, \lambda_2, \lambda_3 \in \mathbb{T}. \tag{3.15}$$

`Case 2:` At least two of $\lambda_1, \lambda_2, \lambda_3$ are same.

Without loss of generality, let's take $\lambda_1 = \lambda_3$ and $\lambda_2 \neq \lambda_3$. Then

$$\varphi[\lambda_1, \lambda_2, \lambda_3] = \frac{1}{(\lambda_1 - \lambda_2)} \varphi'(\lambda_1) - \frac{1}{(\lambda_1 - \lambda_2)^2} \int_{\lambda_2}^{\lambda_1} \varphi'(\xi) d\xi. \tag{3.16}$$

Because of the absolute continuity of φ', integration by parts is valid in (3.16), with φ' to be differentiated and 1 to be integrated with respect to ξ. We thereby immediately obtain

$$\varphi[\lambda_1, \lambda_2, \lambda_3] = \frac{1}{(\lambda_1 - \lambda_2)^2} \int_{\lambda_2}^{\lambda_1} (\xi - \lambda_2) \varphi''(\xi) d\xi, \tag{3.17}$$

By applying [11, Lemma 2.2] to (3.17), we derive the following inequality,

$$|\varphi[\lambda_1, \lambda_2, \lambda_3]| \leq \left(\frac{\pi}{2}\right) \left\| \frac{\partial^2 f}{\partial z_j^2} \right\|_\infty \quad \text{for all } \lambda_1, \lambda_2, \lambda_3 \in \mathbb{T} \text{ and } \lambda_2 \neq \lambda_3. \tag{3.18}$$

Finally, if all $\lambda_1, \lambda_2, \lambda_3$ are equal, then the estimate (3.18) holds trivially.

Combining `Case 1` and `Case 2` we have

$$\left| f(z_1, \dots, z_{j-1}, [\lambda_1, \lambda_2, \lambda_3], z_{j+1}, \dots, z_n) \right| \leq \left(\frac{\pi}{2}\right) \left\| \frac{\partial^2 f}{\partial z_j^2} \right\|_\infty$$

for all $z_1, \dots, z_n, \lambda_1, \lambda_2, \lambda_3 \in \mathbb{T}$. This completes the proof the lemma.

□

Finally, we conclude this section with the following lemma. For notational convenience, we define, for $k_1, \dots, k_n \in \mathbb{Z}$,

$$\|k\| = \max\{|k_1|, \dots, |k_n|\}. \tag{3.19}$$

Lemma 3.5. *Let $N \in \mathbb{N}$ and*

$$\mathcal{P}_N(z_1, \dots, z_n) = \sum_{k \in \mathbb{Z}^n, \|k\| \leq N} c_{k,N} \, z_1^{k_1} \cdots z_n^{k_n},$$

where $c_{k,N}$ is a constant that depends on k and N.

(i) *If* $\lambda, \mu \in \mathbb{T}$, *then*

$$\begin{aligned}&\mathcal{P}_N\left(z_1, \dots, z_{j-1}, [\lambda, \lambda, \mu], z_{j+1}, \dots, z_n\right)\\ &= \sum_{k\in\mathbb{Z}^n, \|k\|\leq N} c_{k,N}\, z_1^{k_1}\cdots z_{j-1}^{k_{j-1}}\Bigg[\sum_{\substack{\alpha_0,\alpha_1,\alpha_2\geq 0\\ \alpha_0+\alpha_1+\alpha_2=k_j-2;\, k_j\geq 2}} \lambda^{(\alpha_0+\alpha_2)}\mu^{\alpha_1}\\ &\quad + \sum_{\substack{\alpha_0,\alpha_1,\alpha_2\geq 0\\ \alpha_0+\alpha_1+\alpha_2=|k_j|-1;\, k_j\leq -1}} \lambda^{-(\alpha_0+\alpha_2+2)}\mu^{-(\alpha_1+1)}\Bigg] z_{j+1}^{k_{j+1}}\cdots z_n^{k_n}.\end{aligned}$$

(ii) *If* $\lambda_1, \lambda_2, \mu_1, \mu_2 \in \mathbb{T}$, *then*

$$\begin{aligned}&\mathcal{D}^{i,j}_{[\lambda_1,\lambda_2],[\mu_1,\mu_2]}\mathcal{P}_N(z_1,\dots,z_n) = \sum_{k\in\mathbb{Z}^n,\|k\|\leq N} c_{k,N}\prod_{l=1}^{i-1} z_l^{k_l}\\ &\times\Bigg[\sum_{\substack{\alpha_0,\alpha_1\geq 0\\ \alpha_0+\alpha_1=k_i-1;\, k_i\geq 1}} \lambda_1^{\alpha_0}\lambda_2^{\alpha_1} - \sum_{\substack{\alpha_0,\alpha_1\geq 0\\ \alpha_0+\alpha_1=|k_i|-1;\, k_i\leq -1}} \lambda_1^{-\alpha_0-1}\lambda_2^{-\alpha_1-1}\Bigg]\prod_{l=i+1}^{j-1} z_l^{k_l}\\ &\times\Bigg[\sum_{\substack{\beta_0,\beta_1\geq 0\\ \beta_0+\beta_1=k_j-1;\, k_j\geq 1}} \mu_1^{\beta_0}\mu_2^{\beta_1} - \sum_{\substack{\beta_0,\beta_1\geq 0\\ \beta_0+\beta_1=|k_j|-1;\, k_j\leq -1}} \mu_1^{-\beta_0-1}\mu_2^{-\beta_1-1}\Bigg]\prod_{l=j+1}^{n} z_l^{k_l}.\end{aligned}$$

Proof. Both the formulas can be proved analogously to [29, Lemma 4.3] for $(k_1, \dots, k_n) \in \mathbb{Z}_+^n$. In contrast, the case $(k_1, \dots, k_n) \in \mathbb{Z}^n \setminus \mathbb{Z}_+^n$ requires some care. Indeed, one applies the following representation to obtain the desired identity:

$$\varphi[\lambda_0, \dots, \lambda_m] = (-1)^m\Bigg[\sum_{\substack{\alpha_0,\dots,\alpha_m\geq 0\\ \alpha_0+\cdots+\alpha_m=\alpha-1}} \lambda_0^{-\alpha_0-1}\lambda_1^{-\alpha_1-1}\cdots\lambda_m^{-\alpha_m-1}\Bigg],$$

for $\varphi(z) = z^{-\alpha}$ with $\alpha \in \mathbb{N}$ and $\lambda_0, \dots, \lambda_m \in \mathbb{T}$. □

4. Proof of Theorem 1.1

The goal of this section is to prove Theorem 1.1. For the reader's convenience, we restate the theorem here. Recall the notation introduced in (1.5).

Theorem 1.1. *Let* $\mathcal{M}_\psi$ *be the Lorentz ideal and suppose the function* ψ *satisfies* (2.3) *for some* $0 < \varepsilon < 1/2$*. Let* τ_ψ *be a bounded singular trace on it. Consider two n-tuple of operators* $\boldsymbol{U}_n$ *and* $\boldsymbol{A}_n$ *such that* $U_j \in \mathcal{U}(\mathcal{H})$ *and* $A_j = A_j^* \in \mathcal{M}_\psi$ *for* $j = 1, \dots, n$*. Suppose that* $\boldsymbol{U}_n \in \mathrm{Com}_n$*. Then, there exist measures* $\mu_1, \dots, \mu_n$ *on* $\mathbb{T}^n$ *such that*

$$\|\mu_j\| \leq \|\tau_\psi\|_{\mathcal{M}_\psi^*}\|A_j\|_{\mathcal{M}_\psi},\ 1 \leq j \leq n \tag{4.1}$$

and

$$\tau_\psi\{\mathcal{R}_1(f, \boldsymbol{U}_n, \boldsymbol{A}_n)\} = \sum_{j=1}^n \int_{\mathbb{T}^n} \frac{\partial f}{\partial z_j}(z_1, \dots, z_n)\, d\mu_j(z_1, \dots, z_n), \tag{4.2}$$

for every $f \in \mathcal{F}_2(\mathbb{T}^n)$.

Proof. From Theorem 3.3(i) we have

$$\frac{d}{ds}\bigg|_{s=0} f(\mathbf{U}_n(s)) = \sum_{j=1}^{n} D_j^f(0). \tag{4.3}$$

Using (4.3), (3.4), Lemma 3.2, cyclicity of the trace, and the pairwise commutativity of the operators $U_1, \dots, U_n$, we derive (see (2.1) for the notation used below)

$$\begin{aligned}
&\tau_\psi\left(\frac{d}{ds}\bigg|_{s=0} f(\mathbf{U}_n(s))\right)\\
&= \sum_{j=1}^{n} \sum_{\substack{(k_1,\dots,k_{j-1},k_{j+1},\dots,k_n)\in\mathbb{Z}^{n-1}\\ k_j>0}} \widehat{f}(k)\,\tau_\psi\{k_j\big(T_{k_1,\dots,k_n}(0)\big)i\,A_j\}\\
&\qquad - \sum_{j=1}^{n} \sum_{\substack{(k_1,\dots,k_{j-1},k_{j+1},\dots,k_n)\in\mathbb{Z}^{n-1}\\ k_j<0}} \widehat{f}(k)\,\tau_\psi\{|k_j|\big(T_{k_1,\dots,k_n}(0)\big)i\,A_j\}\\
&= \sum_{j=1}^{n} \tau_\psi\Big\{\sum_{k\in\mathbb{Z}^n} k_j\widehat{f}(k)\,T_{k_1,\dots,k_{j-1}}(0)\,U_j^{k_j-1}T_{k_{j+1},\dots,k_n}(0)\,U_j\,iA_j\Big\}\\
&= \sum_{j=1}^{n} \tau_\psi\left(\frac{\partial f}{\partial z_j}(\mathbf{U}_n)\,U_j\,iA_j\right).
\end{aligned} \tag{4.4}$$

Thus, by (2.8), we have the following estimate for all $1 \le j \le n$,

$$\left|\tau_\psi\left(\frac{\partial f}{\partial z_j}(\mathbf{U}_n)\,U_j\,iA_j\right)\right| \le \|\tau_\psi\|_{\mathcal{M}_\psi^*}\|A_j\|_{\mathcal{M}_\psi}\cdot\left\|\frac{\partial f}{\partial z_j}\right\|_\infty. \tag{4.5}$$

On the other hand, it is easy to verify that

$$\mathcal{R}_2(f,\mathbf{U}_n,\mathbf{A}_n) \in \mathcal{M}_\psi^2$$

for $f \in \mathcal{F}_2(\mathbb{T}^n)$. As a result, using the fact that $0 < \varepsilon < 1/2$ and from (2.4), we deduce that

$$\tau_\psi\{\mathcal{R}_2(f,\mathbf{U}_n,\mathbf{A}_n)\} = 0,$$

which together with (4.4) further implies

$$\tau_\psi\{\mathcal{R}_1(f,\mathbf{U}_n,\mathbf{A}_n)\} = \sum_{j=1}^{n}\tau_\psi\left(\frac{\partial f}{\partial z_j}(\mathbf{U}_n)\,U_j\,iA_j\right). \tag{4.6}$$

Now from (4.5) and (4.6), using the Riesz-Markov representation and Hahn-Banach theorems, we establish the existence of measures $\mu_1, \dots, \mu_n$ on $\mathbb{T}^n$, satisfying (4.1) and (4.2). This completes the proof. □

5. Proof of Theorem 1.2

In this section, we will go a step further and establish the existence of second order spectral shift measures for n-tuple of commuting unitaries. The main technical ingredient of the proof of Theorem 1.2 is the following estimate.

Theorem 5.1. *Let $\mathcal{M}_\psi$ be the Lorentz ideal, and let τ_ψ be a bounded singular trace on it. Suppose that the Jordan decomposition of τ_ψ is given by $\tau_\psi = \tau_{1,\psi} - \tau_{2,\psi} + i\tau_{3,\psi} - i\tau_{4,\psi}$, where $\tau_{k,\psi}$ (for $1 \le k \le 4$) are the positive components of τ_ψ. Consider two n-tuple of operators, $\boldsymbol{U}_n$ and $\boldsymbol{A}_n$, such that $U_j \in \mathcal{U}(\mathcal{H})$ and $A_j = A_j^* \in \mathcal{M}_\psi^{1/2}$ for $j = 1, \dots, n$. Suppose that there exists $t \in [0,1]$ such that $\boldsymbol{U}_n(t) \in \mathrm{Com}_n$. Then, for every $f \in \mathcal{F}_3(\mathbb{T}^n)$, the following estimate holds:*

$$\left|\tau_\psi\left(D^f_{i,j}(t)\right)\right| \le \begin{cases} \displaystyle\sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*}\left(\frac{\pi}{2}\right)^2 \|A_i\|_{\mathcal{M}_\psi^{1/2}}\|A_j\|_{\mathcal{M}_\psi^{1/2}}\left\|\frac{\partial^2 f}{\partial z_i \partial z_j}\right\|_\infty, & i<j,\\ \displaystyle\sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*}\|A_j\|^2_{\mathcal{M}_\psi^{1/2}}\left[\pi\cdot\left\|\frac{\partial^2 f}{\partial z_j^2}\right\|_\infty + \left\|\frac{\partial f}{\partial z_j}\right\|_\infty\right], & i=j, \end{cases} \tag{5.1}$$

where $D^f_{i,j}(t)$ is given by (3.6) for $1 \le i < j \le n$, and by (3.7) for $1 \le i = j \le n$.

Proof. Let $N \in \mathbb{N}$ and consider

$$\mathcal{P}_N(z_1, \dots, z_n) = \sum_{k \in \mathbb{Z}^n, \|k\| \le N} \left(1 - \frac{\|k\|}{N}\right) \hat{f}(k)\, z_1^{k_1} \cdots z_n^{k_n}, \tag{5.2}$$

where $\|k\| = \max\{|k_1|, \dots, |k_n|\}$. For convenience, we will now denote $c_{k,N} = \left(1 - \frac{\|k\|}{N}\right)\hat{f}(k)$. Then, by [32, Theorem 6.2],

$$\|\mathcal{D}^\alpha \mathcal{P}_N - \mathcal{D}^\alpha f\|_\infty \underset{N\to\infty}{\longrightarrow} 0 \quad \text{for } \alpha = 0,1,2 \tag{5.3}$$

(see (2.6) for the notation). Since

$$\left\|D^f_{i,j}(t)\right\|_{\mathcal{M}_\psi} \le \sum_{k \in \mathbb{Z}^n} \left|k_i k_j \hat{f}(k)\right| \|A_i\|_{\mathcal{M}_\psi^{1/2}}\|A_j\|_{\mathcal{M}_\psi^{1/2}} < \infty,$$

and

$$\begin{aligned} &\sum_{k \in \mathbb{Z}^n, \|k\| \le N} \frac{\|k\|}{N}\left|k_i k_j \hat{f}(k)\right| \|A_i\|_{\mathcal{M}_\psi^{1/2}}\|A_j\|_{\mathcal{M}_\psi^{1/2}}\\ &\quad\le \frac{1}{N}\cdot \sum_{k \in \mathbb{Z}^n, \|k\| \le N} \{|k_1| + \cdots + |k_n|\}\left|k_i k_j \hat{f}(k)\right| \|A_i\|_{\mathcal{M}_\psi^{1/2}}\|A_j\|_{\mathcal{M}_\psi^{1/2}}\\ &\quad\underset{N\to\infty}{\longrightarrow} 0, \end{aligned}$$

a brief computation yields

$$D_{i,j}^{\mathcal{P}_N}(t) \xrightarrow[\mathrm{N}\to\infty]{\|\cdot\|_{\mathcal{M}_\psi}} D_{i,j}^{f}(t),\ 1 \le i \le j \le n.$$

Therefore

$$\tau_\psi\left(D_{i,j}^{f}(t)\right) = \lim_{N\to\infty} \tau_\psi\left(D_{i,j}^{\mathcal{P}_N}(t)\right),\ 1 \le i \le j \le n. \tag{5.4}$$

Hence, it is enough to prove (5.1) for the function $\mathcal{P}_N$. The proof is divided into two cases.

`Case 1:`$(1 \le i < j \le n)$. From (3.6) we derive (see (2.1) for the notation used below)

$$D_{i,j}^{\mathcal{P}_N}(t) = \sum_{k\in\mathbb{Z}^n, \|k\|\le N} c_{k,N}\, T_{k_1,\dots,k_{i-1}}(t) \frac{d}{ds}\Big|_{s=t} U_i(s)^{k_i} T_{k_{i+1},\dots,k_{j-1}}(t) \times \frac{d}{ds}\Big|_{s=t} U_j(s)^{k_j} T_{k_{j+1},\dots,k_n}(t).$$

By Lemma 3.2 it follows that

$$\begin{aligned} &D_{i,j}^{\mathcal{P}_N}(t) \\ &= \sum_{k\in\mathbb{Z}^n, \|k\|\le N} c_{k,N}\, T_{k_1,\dots,k_{i-1}}(t) \Bigg[\sum_{\substack{\alpha_0,\alpha_1\ge 0\\ \alpha_0+\alpha_1=k_i-1;\, k_i\ge 1}} U_i(t)^{\alpha_0}(iA_i)U_i(t)^{\alpha_1+1} \\ &\qquad - \sum_{\substack{\alpha_0,\alpha_1\ge 0\\ \alpha_0+\alpha_1=|k_i|-1;\, k_i\le -1}} U_i(t)^{-\alpha_0-1}(iA_i)U_i(t)^{-\alpha_1} \Bigg] T_{k_{i+1},\dots,k_{j-1}}(t) \\ &\quad \times \Bigg[\sum_{\substack{\beta_0,\beta_1\ge 0\\ \beta_0+\beta_1=k_j-1;\, k_j\ge 1}} U_j(t)^{\beta_0}(iA_j)U_j(t)^{\beta_1+1} \\ &\qquad - \sum_{\substack{\beta_0,\beta_1\ge 0\\ \beta_0+\beta_1=|k_j|-1;\, k_j\le -1}} U_j(t)^{-\beta_0-1}(iA_j)U_j(t)^{-\beta_1} \Bigg] T_{k_{j+1},\dots,k_n}(t). \end{aligned}$$

Let $\mathbf{U}_n(t) \in \mathrm{Com}_n$ for a fixed $t \in [0,1]$. Then, the tracial property of τ_ψ and the pairwise commutativity of the tuple $\mathbf{U}_n(t)$ further imply that

$$\begin{aligned} &\tau_\psi\left(D_{i,j}^{\mathcal{P}_N}(t)\right) \\ &= \sum_{k\in\mathbb{Z}^n, \|k\|\le N} c_{k,N}\, \tau_\psi \Bigg[- \sum_{\substack{\alpha_0,\alpha_1\ge 0\\ \alpha_0+\alpha_1=k_i-1; k_i\ge 1}} \sum_{\substack{\beta_0,\beta_1\ge 0\\ \beta_0+\beta_1=k_j-1; k_j\ge 1}} S_{k_i\ge 1,\, k_j\ge 1}(t) \\ &\qquad + \sum_{\substack{\alpha_0,\alpha_1\ge 0\\ \alpha_0+\alpha_1=k_i-1; k_i\ge 1}} \sum_{\substack{\beta_0,\beta_1\ge 0\\ \beta_0+\beta_1=|k_j|-1; k_j\le -1}} S_{k_i\ge 1,\, k_j\le -1}(t) \end{aligned}$$

$$+ \sum_{\substack{\alpha_0,\alpha_1\geq 0\\ \alpha_0+\alpha_1=|k_i|-1;k_i\leq -1}} \sum_{\substack{\beta_0,\beta_1\geq 0\\ \beta_0+\beta_1=k_j-1;k_j\geq 1}} S_{k_i\leq -1,\,k_j\geq 1}(t)$$
$$- \sum_{\substack{\alpha_0,\alpha_1\geq 0\\ \alpha_0+\alpha_1=|k_i|-1;k_i\leq -1}} \sum_{\substack{\beta_0,\beta_1\geq 0\\ \beta_0+\beta_1=|k_j|-1;k_j\leq -1}} S_{k_i\leq -1,\,k_j\leq -1}(t)\Bigg], \tag{5.5}$$

where

$$\begin{aligned} S_{k_i\geq 1,\,k_j\geq 1}(t) &= T_{k_1,\dots,k_{i-1}}(t)U_i(t)^{\alpha_0}U_j(t)^{\beta_1}T_{k_{j+1},\dots,k_n}(t)\,[A_iU_i(t)]\\ &\quad\times U_i(t)^{\alpha_1}T_{k_{i+1},\dots,k_{j-1}}(t)U_j(t)^{\beta_0}\,[A_jU_j(t)],\\ S_{k_i\geq 1,\,k_j\leq -1}(t) &= T_{k_1,\dots,k_{i-1}}(t)U_i(t)^{\alpha_0}U_j(t)^{-\beta_1-1}T_{k_{j+1},\dots,k_n}(t)\,[A_iU_i(t)]\\ &\quad\times U_i(t)^{\alpha_1}T_{k_{i+1},\dots,k_{j-1}}(t)U_j(t)^{-\beta_0-1}\,[A_jU_j(t)],\\ S_{k_i\leq -1,\,k_j\geq 1}(t) &= T_{k_1,\dots,k_{i-1}}(t)U_i(t)^{-\alpha_0-1}U_j(t)^{\beta_1}T_{k_{j+1},\dots,k_n}(t)\,[A_iU_i(t)]\\ &\quad\times U_i(t)^{-\alpha_1-1}T_{k_{i+1},\dots,k_{j-1}}(t)U_j(t)^{\beta_0}\,[A_jU_j(t)],\\ S_{k_i\leq -1,\,k_j\leq -1}(t) &= T_{k_1,\dots,k_{i-1}}(t)U_i(t)^{-\alpha_0-1}U_j(t)^{-\beta_1-1}T_{k_{j+1},\dots,k_n}(t)\,[A_iU_i(t)]\\ &\quad\times U_i(t)^{-\alpha_1-1}T_{k_{i+1},\dots,k_{j-1}}(t)U_j(t)^{-\beta_0-1}[A_jU_j(t)]. \end{aligned}$$

Let $E_{t,j}$ be the spectral measure of $U_j(t)$ and E_t be the joint spectral measure of the tuple $\mathbf{U}_n(t)$. Then, by the spectral theorem, we have

$$U_j(t)^\alpha = \int_{\mathbb{T}} z^\alpha dE_{t,j}(z), \qquad \alpha\in\mathbb{Z}. \tag{5.6}$$

Let $E_{t,i,\dots,j}$ be the spectral measure defined by

$$E_{t,i,\dots,j}(S_i,\dots,S_j) = E_t\left(\mathbb{C}\times\cdots\times\mathbb{C}\times S_i\times\cdots\times S_j\times\mathbb{C}\times\cdots\times\mathbb{C}\right).$$

Therefore, we have

$$U_i(t)^\alpha T_{k_{i+1},\dots,k_{j-1}}(t)U_j(t)^\beta = \int_{\mathbb{T}^{j-i+1}} z_i^\alpha z_{i+1}^{k_{i+1}}\cdots z_{j-1}^{k_{j-1}} z_j^\beta dE_{t,i,\dots,j}(z_i,\dots,z_j). \tag{5.7}$$

For every $1\leq l\leq n$, there is a sequence of Borel partitions $(\delta_{m,l,\eta_l})_{1\leq\eta_l\leq m}$ of $\mathbb{T}$, a sequence of complex numbers $(z_{m,l,\eta_l})_{1\leq\eta_l\leq m}$, and, for every integer $i\leq p\leq j$, there is a sequence of partitions $(\widetilde{\delta}_{m,p,\gamma_p})_{1\leq\gamma_p\leq m}$ of $\mathbb{T}$ and a sequence of complex numbers $(\widetilde{z}_{m,p,\gamma_p})_{1\leq\gamma_p\leq m}$, from which, using Lemma 3.5(ii) and applying a similar approach from [29, Theorem 4.6] to equation (5.5), we conclude that

$$\begin{aligned} \tau_\psi\left(D_{i,j}^{\mathcal{P}_N}(t)\right) = -\lim_{m\to\infty} \sum_{1\leq\eta_1,\dots,\eta_n,\gamma_i,\dots,\gamma_j\leq m} \Bigg[\mathcal{D}^{i,j}_{[z_{m,i,\eta_i},\widetilde{z}_{m,i,\gamma_i}],[\widetilde{z}_{m,j,\gamma_j},z_{m,j,\eta_j}]}\\ \mathcal{P}_N\big(z_{m,1,\eta_1},\dots,z_{m,i-1,\eta_{i-1}},z,\widetilde{z}_{m,i+1,\gamma_{i+1}},\dots,\widetilde{z}_{m,j-1,\gamma_{j-1}},w,\\ z_{m,j+1,\eta_{j+1}},\dots,z_{m,n,\eta_n}\big)\\ \times\tau_\psi\Big(E_t\left(\delta_{m,1,\eta_1}\times\cdots\times\delta_{m,n,\eta_n}\right)[A_iU_i(t)] \end{aligned}$$

$$E_{t,i,\dots,j}\left(\widetilde{\delta}_{m,i,\gamma_i}\times\cdots\times\widetilde{\delta}_{m,j,\gamma_j}\right)[A_jU_j(t)]\Big)\Big]. \tag{5.8}$$

At this point, we recall the following Jordan decomposition of τ_ψ from [21, Theorem 4.2.2]:

$$\tau_\psi=\tau_{1,\psi}-\tau_{2,\psi}+i\tau_{3,\psi}-i\tau_{4,\psi},$$

where each component is a positive bounded trace on $\mathcal{M}_\psi$. Hence, by applying (3.10) and [6, Lemma 4.6] to (5.8) we finally arrive at

$$\begin{aligned}
&\left|\tau_\psi\left(D_{i,j}^{\mathcal{P}_N}(t)\right)\right|\\
&\leq\left(\frac{\pi}{2}\right)^2\sum_{k=1}^{4}\left(\tau_{k,\psi}\left(\left|A_iU_i(t)\right|^2\right)\right)^{1/2}\left(\tau_{k,\psi}\left(\left|A_jU_j(t)\right|^2\right)\right)^{1/2}\left\|\frac{\partial^2\mathcal{P}_N}{\partial z_i\partial z_j}\right\|_\infty\\
&\leq\left(\frac{\pi}{2}\right)^2\sum_{k=1}^{4}\|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*}\|A_i\|_{\mathcal{M}_\psi^{1/2}}\|A_j\|_{\mathcal{M}_\psi^{1/2}}\left\|\frac{\partial^2\mathcal{P}_N}{\partial z_i\partial z_j}\right\|_\infty.
\end{aligned}\tag{5.9}$$

Thus, (5.9) establishes the estimate (5.1) for $1\leq i<j\leq n$.

`Case 2:`$(1\leq i=j\leq n)$. Again recall that

$$D_{j,j}^{\mathcal{P}_N}(t)=\sum_{k\in\mathbb{Z}^n,\|k\|\leq N}c_{k,N}\,T_{k_1,\dots,k_{j-1}}(t)\,\frac{d^2}{ds^2}\bigg|_{s=t}U_j(s)^{k_j}\,T_{k_{j+1},\dots,k_n}(t),$$

which is same as saying

$$\begin{aligned}
D_{j,j}^{\mathcal{P}_N}(t)=-&\sum_{k\in\mathbb{Z}^n,\|k\|\leq N}c_{k,N}\,T_{k_1,\dots,k_{j-1}}(t)\\
\times\Bigg[-&\sum_{\substack{\alpha_0,\alpha_1\geq0\\ \alpha_0+\alpha_1=|k_j|-1;\,k_j\leq-1}}U_j(t)^{-\alpha_0-1}A_j^2U_j(t)^{-\alpha_1}\\
&+2\sum_{\substack{\alpha_0,\alpha_1,\alpha_2\geq0\\ \alpha_0+\alpha_1+\alpha_2=|k_j|-1;\,k_j\leq-1}}U_j(t)^{-\alpha_0-1}A_jU_j(t)^{-\alpha_1}A_jU_j(t)^{-\alpha_2}\\
&+\sum_{\substack{\alpha_0,\alpha_1\geq0\\ \alpha_0+\alpha_1=k_j-1;\,k_j\geq1}}U_j(t)^{\alpha_0}A_j^2U_j(t)^{\alpha_1+1}\\
&+2\sum_{\substack{\alpha_0,\alpha_1,\alpha_2\geq0\\ \alpha_0+\alpha_1+\alpha_2=k_j-2;\,k_j\geq2}}U_j(t)^{\alpha_0}A_jU_j(t)^{\alpha_1+1}A_jU_j(t)^{\alpha_2+1}\Bigg]T_{k_{j+1},\dots,k_n}(t).
\end{aligned}\tag{5.10}$$

The last equality follows from Lemma 3.2. Due to the pairwise commutativity of the tuple $\mathbf{U}_n(t)$ and the tracial property of τ_ψ, (5.10) further reduces to

$$\tau_\psi\left(D_{j,j}^{\mathcal{P}_N}(t)\right)=\mathtt{S}_{1,N}(t)+\mathtt{S}_{2,N}(t), \tag{5.11}$$

where

$$\mathtt{S}_{1,N}(t) = -2 \sum_{k\in\mathbb{Z}^n, \|k\|\leq N} c_{k,N}\, \tau_\psi\Big[\sum_{\substack{\alpha_0,\alpha_1,\alpha_2\geq 0\\ \alpha_0+\alpha_1+\alpha_2=|k_j|-1;\, k_j\leq -1}} S'_{k_j\leq -1}(t) + \sum_{\substack{\alpha_0,\alpha_1,\alpha_2\geq 0\\ \alpha_0+\alpha_1+\alpha_2=k_j-2;\, k_j\geq 2}} S'_{k_j\geq 2}(t)\Big]$$

and

$$\mathtt{S}_{2,N}(t) = - \sum_{k\in\mathbb{Z}^n, \|k\|\leq N} c_{k,N}\, \tau_\psi\Big[\sum_{\substack{\alpha_0,\alpha_1\geq 0\\ \alpha_0+\alpha_1=k_j-1; k_j\geq 1}} S_{k_j\geq 1}(t) - \sum_{\substack{\alpha_0,\alpha_1\geq 0\\ \alpha_0+\alpha_1=|k_j|-1; k_j\leq -1}} S_{k_j\leq -1}(t)\Big], \tag{5.12}$$

with

$$\begin{aligned} S'_{k_j\leq -1}(t) &= T_{k_1,\dots,k_{j-1}}(t)\, U_j(t)^{-(\alpha_0+\alpha_2+2)}\, T_{k_{j+1},\dots,k_n}(t)\, [A_jU_j(t)] \\ &\qquad \times U_j(t)^{-(\alpha_1+1)}\, [A_jU_j(t)], \\ S'_{k_j\geq 2}(t) &= T_{k_1,\dots,k_{j-1}}(t)\, U_j(t)^{(\alpha_0+\alpha_2)}\, T_{k_{j+1},\dots,k_n}(t)[A_jU_j(t)] \\ &\qquad \times U_j(t)^{\alpha_1}\, [A_jU_j(t)], \\ S_{k_j\geq 1}(t) &= T_{k_1,\dots,k_{j-1}}(t)\, U_j(t)^{(\alpha_0+\alpha_1)}\, T_{k_{j+1},\dots,k_n}(t)\, \left[A_j^2\, U_j(t)\right], \\ S_{k_j\leq -1}(t) &= T_{k_1,\dots,k_{j-1}}(t)\, U_j(t)^{-(\alpha_0+\alpha_1+2)}\, T_{k_{j+1},\dots,k_n}(t)\, \left[A_j^2 U_j(t)\right]. \end{aligned}$$

`Claim 1:`

$$\left|\mathtt{S}_{1,N}(t)\right| \leq \pi \cdot \sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*} \|A_j\|^2_{\mathcal{M}_\psi^{1/2}} \left\| \frac{\partial^2 \mathcal{P}_N}{\partial z_j^2} \right\|_\infty \quad \forall\, N\in\mathbb{N}. \tag{5.13}$$

Similarly as in `Case 1`, for every $1 \leq l \leq n$, there is a sequence of Borel partitions $(\delta_{m,l,\eta_l})_{1\leq \eta_l\leq m}$ of $\mathbb{T}$, a sequence of complex numbers $(z_{m,l,\eta_l})_{1\leq\eta_l\leq m}$, and also a sequence of partitions $(\widetilde{\delta}_{m,\gamma})_{1\leq\gamma\leq m}$ of $\mathbb{T}$ and a sequence of complex numbers $(\widetilde{z}_{m,\gamma})_{1\leq\gamma\leq m}$ along with employing Lemma 3.5(i) to the sum $\mathtt{S}_{1,N}(t)$ we arrive at

$$\begin{aligned} \mathtt{S}_{1,N}(t) = -2 \lim_{m\to\infty} \sum_{1\leq\eta_1,\dots,\eta_n,\gamma\leq m} & \mathcal{P}_N\Big(z_{m,1,\eta_1}, \dots, z_{m,j-1,\eta_{j-1}}, \\ & \left[z_{m,j,\eta_j}, z_{m,j,\eta_j}, \widetilde{z}_{m,\gamma}\right], z_{m,j+1,\eta_{j+1}}, \dots, z_{m,n,\eta_n}\Big) \\ \times \tau_\psi\left(E_t\left(\delta_{m,1,\eta_1}\times\cdots\times\delta_{m,n,\eta_n}\right)[A_jU_j(t)]\, E_{t,j}(\widetilde{\delta}_{m,\gamma})\, [A_jU_j(t)]\right). \end{aligned} \tag{5.14}$$

Finally, applying (3.11) and [6, Lemma 4.6] to (5.14) yields

$$\left|\mathrm{S}_{1,N}(t)\right| \leq \pi \cdot \sum_{k=1}^{4} \tau_{k,\psi}\left(\left|A_j U_j(t)\right|^2\right)\left\|\frac{\partial^2 \mathcal{P}_N}{\partial z_j^2}\right\|_\infty,$$

which immediately proves `Claim 1`.
`Claim 2`:

$$\left|\mathrm{S}_{2,N}(t)\right| \leq \sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*} \left\|A_j\right\|^2_{\mathcal{M}_\psi^{1/2}} \left\|\frac{\partial \mathcal{P}_N}{\partial z_j}\right\|_\infty \quad \forall\, N \in \mathbb{N}. \tag{5.15}$$

In view of (5.12), we have

$$\begin{aligned}
&\mathrm{S}_{2,N}(t)\\
&= -\sum_{\substack{k\in\mathbb{Z}^n,\|k\|\leq N\\ k_j>0}} c_{k,N}\tau_\psi\left\{k_j\, T_{k_1,\dots,k_{j-1}}(t)\, U_j(t)^{k_j-1}\, T_{k_{j+1},\dots,k_n}(t)\,\left[A_j^2\, U_j(t)\right]\right\}\\
&\quad + \sum_{\substack{k\in\mathbb{Z}^n,\|k\|\leq N\\ k_j<0}} c_{k,N}\tau_\psi\left\{|k_j|\, T_{k_1,\dots,k_{j-1}}(t)\, U_j(t)^{k_j-1}\, T_{k_{j+1},\dots,k_n}(t)\,\left[A_j^2\, U_j(t)\right]\right\},
\end{aligned} \tag{5.16}$$

which further reduces to

$$\mathrm{S}_{2,N}(t) = -\tau_\psi\left\{\frac{\partial \mathcal{P}_N}{\partial z_j}(\mathbf{U}_n(t))\left[A_j^2\, U_j(t)\right]\right\}. \tag{5.17}$$

Finally, (5.17) along with (2.5) establishes (5.15).

Applying (5.13) and (5.15) in (5.11) we immediately obtain

$$\left|\tau_\psi\left(D_{j,j}^{\mathcal{P}_N}(t)\right)\right| \leq \sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*}\, \|A_j\|^2_{\mathcal{M}_\psi^{1/2}}\left[\pi \cdot \left\|\frac{\partial^2 \mathcal{P}_N}{\partial z_j^2}\right\|_\infty + \left\|\frac{\partial \mathcal{P}_N}{\partial z_j}\right\|_\infty\right]. \tag{5.18}$$

This establishes the estimate (5.1) for $1 \leq i = j \leq n$, which completes the proof of the theorem. □

The estimate in the above theorem is crucial for establishing the second order perturbation formula, which is one of the key components of this section. The reader familiar with the work of [29] could easily find similarities between the estimates (5.1) and [29, Theorem 4.6]. Despite the similarity, one can not obtain the estimate (5.1) directly from [29] because [29] deals with linear path in comparison with multiplicative path considered in this article. In other words, establishing these estimates for multiplicative paths is usually more difficult than for linear paths (see the expressions in Lemma 3.2 and in [29, Lemma 3.1]).

We now supply a proof of Theorem 1.2. Again, for the reader's ease, we restate Theorem 1.2 below.

Theorem 1.2. *Let $\mathcal{M}_\psi$ be the Lorentz ideal and suppose the function ψ satisfies (2.3) for some $0 < \varepsilon < 1/3$. Let τ_ψ be a bounded singular trace on it. Consider two n-tuple of operators $\boldsymbol{U}_n$ and $\boldsymbol{A}_n$ such that $U_j \in \mathcal{U}(\mathcal{H})$ and $A_j = A_j^* \in \mathcal{M}_\psi^{1/2}$ for $j = 1, \dots, n$. Suppose that $\boldsymbol{U}_n \in \mathrm{Com}_n$. Then, there exist finite measures μ_{ij}, ν_j for $1 \le i \le j \le n$ on $\mathbb{T}^n$ such that*

$$\tau_\psi\{\mathcal{R}_2(f, \boldsymbol{U}_n, \boldsymbol{A}_n)\} = \sum_{1\le i\le j\le n} \int_{\mathbb{T}^n} \frac{\partial^2 f}{\partial z_i \partial z_j}(z_1, \dots, z_n)\, d\mu_{ij}(z_1, \dots, z_n) + \sum_{1\le j\le n} \int_{\mathbb{T}^n} \frac{\partial f}{\partial z_j}(z_1, \dots, z_n)\, d\nu_j(z_1, \dots, z_n), \tag{5.19}$$

for every $f \in \mathcal{F}_3(\mathbb{T}^n)$.

Proof. Observe that

$$\mathcal{R}_3(f, \mathbf{U}_n, \mathbf{A}_n) \in \mathcal{M}_\psi^{3/2}.$$

Since $0 < \varepsilon < 1/3$, it follows from (2.4) that $\tau_\psi\{\mathcal{R}_3(f, \mathbf{U}_n, \mathbf{A}_n)\} = 0$. Hence, we obtain

$$\tau_\psi\{\mathcal{R}_2(f, \mathbf{U}_n, \mathbf{A}_n)\} = \frac{1}{2}\tau_\psi\left(\frac{d^2}{ds^2}\bigg|_{s=0} f(\mathbf{U}_n(s))\right).$$

From the last equation and (3.5), we derive

$$\tau_\psi\{\mathcal{R}_2(f, \mathbf{U}_n, \mathbf{A}_n)\} = \sum_{1\le i<j\le n} \tau_\psi\left(D^f_{i,j}(0)\right) + \frac{1}{2}\sum_{1\le j\le n} \tau_\psi\left(D^f_{j,j}(0)\right). \tag{5.20}$$

We again recall the following Jordan decomposition of τ_ψ from [21, Theorem 4.2.2]:

$$\tau_\psi = \tau_{1,\psi} - \tau_{2,\psi} + i\tau_{3,\psi} - i\tau_{4,\psi},$$

where each $\tau_{k,\psi}$ $(k = 1, 2, 3, 4)$ is a positive bounded trace on $\mathcal{M}_\psi$.

Next, to proceed, we need to revisit the proof of Theorem 5.1, particularly `Case 2`. Indeed, (3.11) and (5.14) collectively implies that

$$\begin{aligned}\lim_{N\to\infty} \mathtt{S}_{1,N}(0) = -2 \lim_{m\to\infty} &\sum_{1\le \eta_1,\dots,\eta_n,\gamma\le m} f\Big(z_{m,1,\eta_1}, \dots, z_{m,j-1,\eta_{j-1}}, \\ &\left[z_{m,j,\eta_j}, z_{m,j,\eta_j}, \widetilde{z}_{m,\gamma}\right], z_{m,j+1,\eta_{j+1}}, \dots, z_{m,n,\eta_n}\Big) \\ &\times \tau_\psi\left(E_0\left(\delta_{m,1,\eta_1} \times \cdots \times \delta_{m,n,\eta_n}\right)[A_j U_j]\, E_{0,j}(\widetilde{\delta}_{m,\gamma})[A_j U_j]\right) \\ &:= \Gamma_f^{1,j}(0),\end{aligned} \tag{5.21}$$

and

$$\left|\Gamma_f^{1,j}(0)\right| \le \pi \sum_{k=1}^4 \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*} \|A_j\|^2_{\mathcal{M}_\psi^{1/2}} \left\|\frac{\partial^2 f}{\partial z_j^2}\right\|_\infty. \tag{5.22}$$

From (5.17) and (5.3), it is evident that

$$\lim_{N\to\infty} \mathrm{S}_{2,N}(0) = -\tau_\psi \left\{ \frac{\partial f}{\partial z_j}(\mathbf{U}_n(0)) \left[A_j^2 U_j\right] \right\} := \Gamma_f^{2,j}(0), \tag{5.23}$$

with

$$\left|\Gamma_f^{2,j}(0)\right| \le \sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*} \|A_j\|^2_{\mathcal{M}_\psi^{1/2}} \left\| \frac{\partial f}{\partial z_j} \right\|_\infty . \tag{5.24}$$

Hence, by combining (5.4), (5.11), (5.21), and (5.23), we obtain

$$\tau_\psi\left(D^f_{j,j}(0)\right) = \Gamma_f^{1,j}(0) + \Gamma_f^{2,j}(0). \tag{5.25}$$

Finally, applying the Riesz-Markov representation theorem for a bounded linear functional on $C(\mathbb{T}^n)$ and the Hahn-Banach theorem, we deduce from (5.20), (5.25), (5.22), (5.24), and Theorem 5.1 the existence of measures μ_{ij} and ν_j for $1 \le i \le j \le n$ satisfying

$$\tau_\psi\left(D^f_{i,j}(0)\right) = \int_{\mathbb{T}^n} \frac{\partial^2 f}{\partial z_i \partial z_j}(z_1,\dots,z_n)\, d\mu_{ij}(z_1,\dots,z_n), \quad i<j,$$

$$\frac{1}{2}\Gamma_f^{1,j}(0) = \int_{\mathbb{T}^n} \frac{\partial^2 f}{\partial z_j^2}(z_1,\dots,z_n)\, d\mu_{jj}(z_1,\dots,z_n),$$

$$\frac{1}{2}\Gamma_f^{2,j}(0) = \int_{\mathbb{T}^n} \frac{\partial f}{\partial z_j}(z_1,\dots,z_n)\, d\nu_j(z_1,\dots,z_n).$$

This leads to (5.19). Thus, the proof is complete. □

A closer look at the proof of Theorem 1.2 yields additional information about the measures obtained there, which we record in the following remark.

Remark 5.2. Note that the total variation of the measures obtained in Theorem 1.2 can be computed. Moreover, from the final part of the proof of Theorem 1.2, we have

$$\left\|\mu_{ij}\right\| \le \left(\frac{\pi}{2}\right)^2 \sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*} \|A_i\|_{\mathcal{M}_\psi^{1/2}} \left\|A_j\right\|_{\mathcal{M}_\psi^{1/2}}, \quad 1 \le i < j \le n,$$

$$\left\|\mu_{jj}\right\| \le \frac{\pi}{2} \sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*} \left\|A_j\right\|^2_{\mathcal{M}_\psi^{1/2}}, \quad 1 \le j \le n, \quad \text{and}$$

$$\left\|\nu_j\right\| \le \frac{1}{2} \sum_{k=1}^{4} \|\tau_{k,\psi}\|_{\mathcal{M}_\psi^*} \left\|A_j\right\|^2_{\mathcal{M}_\psi^{1/2}}, \quad 1 \le j \le n,$$

where $\tau_{k,\psi}$ ($k = 1,2,3,4$) are the positive components of the Jordan decomposition of τ_ψ.

Finally, it is natural to ask whether Theorems 1.1 and 1.2 can also be established for perturbations from the trace class ideal and the Hilbert–Schmidt ideal, respectively. In fact, with all the necessary estimates in hand (see (4.5) and (5.1), which also hold for $\mathcal{S}^1(\mathcal{H})$ and $\mathcal{S}^2(\mathcal{H})$ perturbations, respectively, with respect to the canonical trace Tr), these results can indeed be obtained using arguments analogous to those in [29], under the more restrictive assumption that $\mathbf{U}_n(t) \in \mathrm{Com}_n$ for every $t \in [0,1]$. Whether the results remain valid when only $\mathbf{U}_n \in \mathrm{Com}_n$ under these ideal perturbations is a question that remains open.

Acknowledgements. The authors would like to heartily thank the anonymous referee for a careful reading of the manuscript and several helpful suggestions. They also gratefully acknowledge useful conversations with Chandan Pradhan. A. Chattopadhyay is supported by the Core Research Grant (CRG), File No: CRG/2023/004826, from SERB. S. Giri is grateful to the Ministry of Education, Government of India, for financial support through the Prime Minister's Research Fellowship (PMRF-ID: 1902164) grant.

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This paper is available via http://nyjm.albany.edu/j/2026/32-21.html.