Commun. Math. Phys. 183, 339–363 (1997)

Communications in
Mathematical
Physics

Quantum Analysis – Non-Commutative Differential and Integral Calculi

Masuo Suzuki

Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan

Received: 20 November 1995 / Accepted: 13 June 1996

Abstract: A new scheme of quantum analysis, namely a non-commutative calculus of operator derivatives and integrals is introduced. This treats differentiation of an operator-valued function with respect to the relevant operator in a Banach space. In this new scheme, operator derivatives are expressed in terms of the relevant operator and its inner derivation explicitly. Derivatives of hyperoperators are also defined. Some possible applications of the present calculus to quantum statistical physics are briefly discussed.

I. Introduction

In theoretical sciences, non-commutative operators play an important role. In particular, the differentiation of an operator $A(t)$ with respect to the relevant parameter t is frequently used. As is well known, the derivative of $A(t)$ is defined by

$$A'(t) \equiv \frac{dA(t)}{dt} = \lim_{h\to 0} \frac{A(t+h) - A(t)}{h} . \tag{1.1}$$

Norm convergence of (1.1) can be discussed in a Banach space and strong convergence is appropriate for unbounded linear operators.

In many situations, we treat an operator-valued function $f(A(t))$ of the operator $A(t)$, such as an exponential operator [1–15] $\exp A(t)$. Since the derivative $A'(t)$ does not commute with $A(t)$ in general, the derivative of $\exp A(t)$ is given by the following integral [1, 3, 5]:

$$\frac{d}{dt} e^{A(t)} = e^{A(t)} \int_0^1 e^{-\lambda A(t)} A'(t) e^{\lambda A(t)}\, d\lambda . \tag{1.2}$$

When $A'(t) \equiv dA(t)/dt$ commutes with $A(t)$, we have

$$\frac{d}{dt} e^{A(t)} = e^{A(t)} \frac{dA(t)}{dt} . \tag{1.3}$$

This may be interpreted formally as

$$\frac{d}{dt}e^{A(t)} = \frac{de^{A(t)}}{dA(t)} \cdot \frac{dA(t)}{dt} . \tag{1.4}$$

Here

$$\frac{de^{A(t)}}{dA(t)} = e^{A(t)} \tag{1.5}$$

when $A'(t)$ commutes with $A(t)$. How about the general situation in which $A'(t)$ does not commute with $A(t)$? One of the motivations of the present paper is to answer this question.

A simple-minded extension of the ordinary differentiation to the operator-valued function $f(A)$ might be given by

$$\lim_{dA \to 0} (f(A + dA) - f(A))(dA)^{-1} \tag{1.6}$$

for a regular operator dA. However, the above limit *is not unique* but depends on how dA approaches zero (operator), as is easily seen in the simple example $f(A) = A^2$, namely

$$\lim_{dA \to 0} ((A + dA)^2 - A^2)(dA)^{-1} = A + \lim_{dA \to 0} (dA)A(dA)^{-1} . \tag{1.7}$$

Clearly, the second term on the right-hand side of (1.7) is not unique. It turns out that (1.5) can not be extended to the noncommutative case, if we restrict the derivative $df(A)/dA$ on an operator space. Thus, we have to consider differentiation of an operator-valued function *with respect to the relevant operator in an extended space, namely a hyperoperator space.*

II. Definition of Operator Derivative

We start with the Gâteaux differential $df(A)$ of $f(A)$ as [1]

$$df(A) = \lim_{h \to 0} \frac{f(A + hdA) - f(A)}{h} \tag{2.1}$$

for $h \in C$ and for a fixed operator dA. When there exists a bounded linear mapping $\mathscr{L}$ satisfying the relation

$$\lim_{B \to 0} \|f(A + B) - f(A) - \mathscr{L}(B)\| \,/\, \|B\| = 0 , \tag{2.2}$$

$\mathscr{L}$ is called the Fréchet derivative [1]. Eq. (1.2) is such an example. The differentiation $df(A)/dA$ of $f(A)$ with respect to A in our quantum analysis will be represented by

$$\frac{df(A)}{dA} = f_1(A, \delta_A); \qquad df(A) = f_1(A, \delta_A) \cdot dA , \tag{2.3}$$

where $f_1(A, \delta_A)$ is expressed in terms of the relevant operator A and the inner derivation δ_A. This is kind of Fréchet derivative. Namely, the derivative $df(A)/dA$ is a *hyperoperator* [1], which maps an arbitrary operator dA to the derivation $df(A)$ defined by (2.1). However, the product structure of (2.3) is crucial in our calculus, as will be seen later. Here we have used a simple notation A to express the left multiplication hyperoperator $L_A : X \to AX$ [1]. Note that the left multiplication hyperoperator L_A and inner derivation hyperoperator δ_A (defined in (2.5) below) commute with each other, namely $\delta_A g(A) \cdot dA = \delta_A g(L_A) \cdot dA = g(L_A)\delta_A \cdot dA = g(A)\delta_A \cdot dA$. Throughout the paper we will not distinguish between L_A and A. Since $f(L_A) = L_{f(A)}$ for any function f, no confusion arises in this way.

In the above simple example $f(A) = A^2$, we have

$$dA^2 = \lim_{h\to 0}((A + hdA)^2 - A^2)/h = A \cdot dA + (dA) \cdot A = (2A - \delta_A) \cdot dA\,, \qquad (2.4)$$

where the inner derivation δ_A is defined by

$$\delta_A \cdot Q \equiv \delta_A(Q) \equiv [A, Q] = AQ - QA\,. \qquad (2.5)$$

Thus, the "operator derivative" of A^2 is given by

$$\frac{dA^2}{dA} = 2A - \delta_A\,. \qquad (2.6)$$

The second term on the right-hand side of (2.6) denotes a new effect due to the noncommutativity of A and dA. We try in the present paper to express the operator derivative $df(A)/dA$ only in terms of A and the inner derivation δ_A as a hyperoperator $f_1(A, \delta_A)$, explicitly, as in the example (2.6). This idea is extended also to higher derivatives and partial derivatives in the Banach algebra. This is a new aspect of the present *quantum analysis*, in comparison with other formulations [1].

III. Basic Formulas and Theorems

We consider first the differential dA^n for a positive integer n, where A belongs to a Banach space. According to the definition (2.1), we have

$$dA^n = \lim_{h\to 0} \frac{(A + hdA)^n - A^n}{h} = \sum_{j=1}^{n} A^{j-1}(dA) \cdot A^{n-j}$$

$$= \left(nA^{n-1} - \sum_{j=1}^{n} A^{j-1}\delta_{A^{n-j}} \right) \cdot dA\,. \qquad (3.1)$$

The limit in (3.1) is defined by the uniform topology in a Banach space. Therefore, we obtain

$$\frac{dA^n}{dA} = nA^{n-1} - \sum_{j=1}^{n} A^{j-1}\delta_{A^{n-j}}\,. \qquad (3.2)$$

This can be rewritten in a compact form using the following formulas.

Formula 1. We have

$$\delta_{f(A)g(A)} = f(A)\delta_{g(A)} + g(A)\delta_{f(A)} - \delta_{g(A)}\delta_{f(A)}\,. \qquad (3.3)$$

In particular, we have

$$\delta_{Ag(A)} = A\delta_{g(A)} + (g(A) - \delta_{g(A)})\delta_A\,. \qquad (3.4)$$

Using Eq. (3.4), we obtain the following formula by induction.

Formula 2. For a positive integer n, we have

$$\delta_{A^n} = A^n - (A - \delta_A)^n\,. \qquad (3.5)$$

The proof is by induction. First we assume (3.5) for a positive integer n. Then, using (3.4) we obtain

$$\delta_{A^{n+1}} = \delta_{A \cdot A^n} = A\delta_{A^n} - \delta_{A^n}\delta_A + A^n\delta_A = A^{n+1} - (A - \delta_A)^{n+1} , \tag{3.6}$$

because $[A, \delta_A] = 0$.

Thus, we arrive at the following formula.

Formula 3. For a positive integer n,

$$\frac{dA^n}{dA} = (A^n - (A - \delta_A)^n)\delta_A^{-1} = \frac{\delta_{A^n}}{\delta_A} . \tag{3.7}$$

Here the notation δ_A^{-1} in (3.7) is rather formal. Since the numerator in (3.7) contains δ_A, the quotient (3.7) is well defined after the cancellation of δ_A and δ_A^{-1}. The proof of Eq. (3.7) is easily given.

The above formula (3.5) can be extended to a more general form.

Formula 4. When $f(x)$ is analytic for $|x - a| < b$, we have

$$\delta_{f(A)} = f(A) - f(A - \delta_A) . \tag{3.8}$$

This is valid for $\|A - a\| < b$ when $\delta_{f(A)}$ is applied to the operator dA in the domain $\mathscr{D}$ defined by

$$\mathscr{D} = \{dA; \|(A - a - \delta_A)^n dA\| < b^n \text{ for all } n \in Z\} . \tag{3.9}$$

The proof is given as follows. First we expand $f(x)$ in a power series (i.e., a Taylor expansion):

$$f(x) = \sum_{n=0}^{\infty} c_n(x - a)^n; \qquad c_n = \frac{1}{n!}f^{(n)}(a) . \tag{3.10}$$

Then, we have

$$\begin{aligned}\delta_{f(A)} &= \sum_{n=0}^{\infty} c_n\delta_{(A-a)^n} = \sum_{n=0}^{\infty} c_n((A - a)^n - (A - a - \delta_A)^n) \\ &= f(A) - f(A - \delta_A) . \end{aligned}\tag{3.11}$$

In general, we easily obtain the following formulas.

Formula 5. When $f(A)$ and $g(A)$ are differentiable, we have

$$\frac{d}{dA}(f(A) + g(A)) = \frac{df(A)}{dA} + \frac{dg(A)}{dA} . \tag{3.12}$$

Formula 6. When $f(A)$ and $g(A)$ are differentiable, we have

$$\frac{d}{dA}(f(A) \cdot g(A)) = (g(A) - \delta_{g(A)})\frac{df(A)}{dA} + f(A)\frac{dg(A)}{dA} . \tag{3.13}$$

Using formulas 3, 4, 5 and 6, we finally arrive at the following theorem.

Theorem I. *When $f(x)$ is analytic for $|x - a| < b$, the derivative $df(A)/dA$ exists uniquely and it is given by*

$$\frac{df(A)}{dA} = \frac{f(A) - f(A - \delta_A)}{\delta_A} = \frac{\delta_{f(A)}}{\delta_A} = \int_0^1 dt f^{(1)}(A - t\delta_A) \tag{3.14}$$

for $\|A - a\| < b$. *This is valid when it is applied to the operator* dA *in the domain* $\mathscr{D}$ *defined by* (3.9). *Equivalently, we have*

$$\delta_{f(A)} = \delta_A \frac{df(A)}{dA}, \quad \text{or} \quad \delta_A df(A) = \delta_{f(A)} \cdot dA \,. \tag{3.15}$$

Proof of Theorem I. First we expand $f(x)$ as a power series in the form (3.10). Then, we obtain

$$\begin{aligned}\frac{df(A)}{dA} \equiv \frac{d}{dA} f(A) &= \sum_{n=0}^{\infty} c_n \frac{d}{dA}(A-a)^n \\ &= \sum_{n=0}^{\infty} c_n((A-a)^n - (A-a-\delta_A)^n)/\delta_A \\ &= (f(A) - f(A-\delta_A))/\delta_A = \frac{\delta_{f(A)}}{\delta_A}\end{aligned} \tag{3.16}$$

in the domain $\mathscr{D}$ defined by (3.9). The convergence of (2.1) for $f(A)$ satisfying the condition in Theorem I is shown as

$$\begin{aligned}&\lim_{h\to 0}\left\| \frac{f(A+hdA) - f(A)}{h} - \frac{f(A) - f(A-\delta_A)}{\delta_A} \cdot dA \right\| \\ &\leqq \lim_{h\to 0}(f_0(\|A-a\| + |h| \cdot \|dA\|) - f_0(\|A-a\|) - |h| \cdot \|dA\| f_1(\|A-a\|))/|h| \\ &\leqq \lim_{h\to 0} \frac{|h|}{2} \|dA\|^2 f_2(\|A-a\| + \theta|h| \cdot \|dA\|) = 0\end{aligned} \tag{3.17}$$

for $0 < \theta < 1$, using the Maclaurin–Taylor theorem. Here, $\{f_j(x)\}$ are defined by

$$f_j(x) = \sum_{n=0}^{\infty} \frac{n!|c_n|}{(n-j)!} x^{n-j}; \quad j = 0, 1, 2 \,, \tag{3.18}$$

which are convergent for $|x| < b$.

It should be instructive to remark here the following theorem.

Theorem II. *When the derivatives* $df(A)/dA$ *and* $dA(t)/dt$ *exist, we have*

$$\frac{d}{dt} f(A(t)) = \frac{df(A(t))}{dA(t)} \cdot \frac{dA(t)}{dt} \,. \tag{3.19}$$

This is almost self-evident from Definition (2.2) with (2.1). Anyway, the proof of (3.19) is easily given as follows. From the condition in (3.19), we may put

$$A(t+h) = A(t) + hA'(t) + hR(h) \,, \tag{3.20}$$

where

$$\lim_{h\to 0} R(h) = 0 \,. \tag{3.21}$$

Then, we obtain

$$\lim_{h\to 0}\frac{f(A(t+h))-f(A(t))}{h}$$

$$=\lim_{h\to 0}\frac{f(A(t)+h(A'(t)+R(h)))-f(A(t))}{h}$$

$$=\frac{df(A(t))}{dA(t)}\cdot\lim_{h\to 0}(A'(t)+R(h))=\frac{df(A(t))}{dA(t)}\cdot\frac{dA(t)}{dt}\,. \tag{3.22}$$

Theorem II is practically very important, as is shown in the following quantum analysis. Concerning the derivative of a function of an operator-valued function, $f(g(A))$, we have the following.

Theorem III. *When the derivatives $df(A)/dA$ and $dg(A)/dA$ exist and are bounded, we have*

$$\frac{df(g(A))}{dA}=\frac{df(g(A))}{dg(A)}\frac{dg(A)}{dA}\,. \tag{3.23}$$

The proof is given as follows. From the conditions in Theorem III, we may put

$$f(g+hdg)=f(g)+hf'(g)\,dg+hR_f(h,dg)\,, \tag{3.24}$$

and

$$g(A+hdA)=g(A)+hg'(A)\,dA+hR_g(h,dA)\,, \tag{3.25}$$

where

$$\lim_{h\to 0}R_f(h,dg)=0 \quad \text{and} \quad \lim_{h\to 0}R_g(h,dA)=0\,. \tag{3.26}$$

Then, we arrive at

$$\left\|\frac{f(g(A+hdA))-f(g(A))}{h}-\frac{df(g(A))}{dg(A)}\frac{dg(A)}{dA}\cdot dA\right\| \leqq \|f'(g(A))\|\cdot\|R_g(h,dA)\|$$

$$+\|R_f(h,g'(A)dA+R_g(h,dA))g'(A)dA+R_g(h,dA)\| \to 0 \text{ as } h\to 0\,. \tag{3.27}$$

Similarly we have the following.

Theorem IV. *Let $f^{-1}(x)$ be the inverse function of $f(x)$. When the derivatives $df(A)/dA$ and $df^{-1}(A)/dA$ exist, we have*

$$\frac{d}{dA}f^{-1}(A)=1\Big/\left(\frac{df(B)}{dB}\right)_{B=f^{-1}(A)}\,. \tag{3.28}$$

This is easily derived by putting $B=f^{-1}(A)$ and by differentiating

$$f(B)=A\,, \tag{3.29}$$

with the use of Theorem III and Formula 3 for $n=1$.

Furthermore, we have the following formulas 7 $\sim$ 12, in a region wider than the domain $\mathscr{D}$ in Theorem I.

Formula 7. We have

$$\frac{d}{dA}A^{-1} = -A^{-2} + A^{-1}\delta_{A^{-1}} . \tag{3.30}$$

Formula 8. For any positive integer n, we have

$$\frac{d}{dA}A^{-n} = -A^{-n}(A^{-n} - \delta_{A^{-n}})\delta_{A^n}\delta_A^{-1} . \tag{3.31}$$

Formula 9. For a positive-definite operator A, we have

$$\frac{d}{dA}\log A = \frac{\log A - \log(A - \delta_A)}{\delta_A} = \frac{\delta_{\log A}}{\delta_A} = \frac{\delta_{\log A}}{1 - e^{-\delta_{\log A}}} \cdot A^{-1}$$
$$= \Delta^{-1}(-\log A) \cdot A^{-1} = -\delta_A^{-1}\log(1 - A^{-1}\delta_A) , \tag{3.32}$$

where

$$\Delta(A) = \frac{e^{\delta_A} - 1}{\delta_A} \quad \text{and} \quad \Delta^{-1}(A) = \frac{\delta_A}{e^{\delta_A} - 1} . \tag{3.33}$$

In deriving (3.32), we have used the following formula.

Formula 10. For a positive-definite operator A, we have

$$e^{\delta_{\log A}} = 1 - A\delta_{A^{-1}} \quad \text{and} \quad e^{-\delta_{\log A}} = 1 - A^{-1}\delta_A . \tag{3.34}$$

Formula 11. When A is a positive-definite operator, we have

$$\frac{d}{dA}A^{1/2} = (A^{1/2} - (A - \delta_A)^{1/2})/\delta_A = (2A^{1/2} - \delta_{A^{1/2}})^{-1} \tag{3.35}$$

for $\|A - a\| < a$.

Formula 12. Using $\Delta(-A)$ in (3.33), we have

$$\frac{d}{dA}e^A = e^A\Delta(-A) . \tag{3.36}$$

Proof. From Theorem I, we have

$$\frac{d}{dA}e^A = (e^A - e^{A-\delta_A})\delta_A^{-1} = e^A(1 - e^{-\delta_A})\delta_A^{-1} = e^A\Delta(-A) . \tag{3.37}$$

This formula can be also derived directly from (1.2) and Theorem II as

$$\frac{d}{dt}e^{A(t)} = e^{A(t)}\int_0^1 e^{-\lambda\delta_{A(t)}}A'(t)d\lambda = e^{A(t)}\Delta(-A(t)) \cdot A'(t) , \tag{3.38}$$

using the identity $e^{\delta_A}B = e^ABe^{-A}$. Formula 12 will be used effectively in deriving higher-order exponential product formulas using the quantum analysis [16].

IV. Higher Derivatives

It is not straightforward to extend the above quantum analysis to higher derivatives, because the first-order derivative $df(A)/dA$ is a hyperoperator which maps dA to $df(A)$.

It is convenient to introduce a higher-level hyperoperator which maps a hyperoperator $df(A)/dA$ to another hyperoperator as

$$\frac{d^2f(A)}{dA^2} : dA \cdot dA = \lim_{h\to 0} \frac{f(A+hdA)+f(A-hdA)-2f(A)}{h^2}$$
$$= \lim_{h\to 0} \frac{f(A+2hdA)+f(A)-2f(A+hdA)}{h^2} . \quad (4.1)$$

In general, the n^{th} order derivative is defined as

$$\frac{d^nf(A)}{dA^n} : \underbrace{dA \cdot - - - - \cdot dA}_{n} = \lim_{h\to 0} \sum_{j=0}^{n} \frac{(-1)^{n-j}}{h^n} \binom{n}{j} f(A+jhdA) . \quad (4.2)$$

By the above notation on the left-hand side of (4.2), we mean that $d^nf(A)/dA^n$ is a hyperoperator in the Banach algebra [1], which maps the set or product of the operators $dA \cdot - - - - \cdot dA$ to the limit on the right-hand side of (4.2). It is given by a hyperoperator-valued function of the operator A and the inner derivations $\delta_A^{(1)}, \delta_A^{(2)}, \ldots, \delta_A^{(n)}$ which operate on each dA of the set $dA \cdot dA \cdot - - - - \cdot dA$ in this order. Using the notation $dA \cdot dA \cdot - - - - \cdot dA \equiv (dA)^n$, the inner derivations $\{\delta_A^{(j)}\}$ are defined more explicitly by

$$\delta_A^{(j)} : (dA)^n = (dA)^{n-j} \cdot (\delta_A dA) \cdot (dA)^{j-1},$$

and

$$f(A) : (dA)^n = f(A)(dA)^n . \quad (4.3)$$

These hyperoperators $\{\delta_A^{(j)}\}$ commute with each other and they are multi-linear hyperoperators.

As in Sect. III, we may first study d^nA^k/dA^n using Definition (4.2), and then we may derive $d^nf(A)/dA^n$. However, this procedure is extremely complicated. We find that an exponential operator e^{tA} is the most basic in quantum analysis. We should explain this remark later. Thus, we derive first the n^{th} derivative $d^n \mathrm{e}^{tA}/dA^n$ and then we calculate d^nA^k/dA^n through the formula

$$\frac{d^nA^k}{dA^n} = \left[\frac{d^k}{dt^k} \left(\frac{d^n \mathrm{e}^{tA}}{dA^n} \right) \right]_{t=0} . \quad (4.4)$$

The n^{th} derivative $d^nf(A)/dA^n$ of a general operator-valued function $f(A)$ will be obtained using the Laplace transformation and the derivative $d^n \mathrm{e}^{tA}/dA^n$, as will be discussed later explicitly. An alternative definition of higher-order derivatives will be given as follows.

Alternative definition of the derivatives $\{d^nf(A)/dA^n\}$. *The n^{th} derivative $d^nf(A)/dA^n$ is defined by*

$$f(A+xB) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{d^nf(A)}{dA^n} : B^n \quad (4.5)$$

in the present representation.

The proof of the equivalence of the two definitions (4.2) and (4.5) is almost evident. Namely, if we expand $f(A+xB)$ as

$$f(A+xB) = \sum_{n=0}^{\infty} \frac{x^n}{n!} f_n(A) : B^n , \tag{4.6}$$

then we find easily

$$f_n(A) = \frac{d^n f(A)}{dA^n} , \tag{4.7}$$

using Definition (4.2). This is because the formal structure of (4.5) is the same as the ordinary Taylor expansion

$$f(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} f^{(n)}(0) . \tag{4.8}$$

An ordinary operator Taylor expansion is given in the form [1, 4]:

$$f(A+xB) = \sum_{n=0}^{\infty} \frac{x^n}{2\pi i} \int_C \frac{f(z)}{z-A} \left(B \frac{1}{z-A} \right)^n dz , \tag{4.9}$$

where $\int_C$ denotes an anti-clockwise integration around the path C. However, this formula contains the operator B in many intermediate places and consequently it is different from our required multiplication form (4.5).

(i) General method for higher derivatives. Now we study the derivative of e^{tA} with respect to the operator A. From the above definition, we have

$$e^{t(A+xB)} = \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{d^n e^{tA}}{dA^n} : B^n . \tag{4.10}$$

On the other hand, we have the following Feynman expansion:

$$e^{t(A+xB)} = e^{tA} + \sum_{n=1}^{\infty} x^n e^{tA} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n B(t_1) \cdots B(t_n) , \tag{4.11}$$

where

$$B(t) = e^{-tA} B e^{tA} = e^{-t\delta_A} \cdot B . \tag{4.12}$$

Thus, we obtain the following formula. Hereafter we make the following abbreviation: $\delta_A^{(j)} \equiv \delta_j$ for a fixed operator A.

Formula 13. We have

$$\frac{d^n e^{tA}}{dA^n} = n!\, e^{tA} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, e^{-t_1\delta_1 - \cdots - t_n\delta_n} . \tag{4.13}$$

Formula 14. In particular, we have

$$\frac{de^{tA}}{dA} = e^{tA} \int_0^t e^{-t_1\delta_1} dt_1 = e^{tA} \left(\frac{1-e^{-t\delta_1}}{\delta_1} \right), \tag{4.14a}$$

and

$$\frac{d^2 e^{tA}}{dA^2} = 2e^{tA} \int_0^t dt_1 \int_0^{t_1} dt_2\, e^{-t_1\delta_1 - t_2\delta_2}$$

$$= 2e^{tA} \left(\frac{1-e^{-t\delta_1}}{\delta_1\delta_2} - \frac{1-e^{-t(\delta_1+\delta_2)}}{(\delta_1+\delta_2)\delta_2} \right) . \tag{4.14b}$$

In order to find an explicit expression of $d^n\,\mathrm{e}^{tA}/dA^n$, we introduce the following function:

$$S_n(\{x_j\};t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, \mathrm{e}^{-t_1x_1-t_2x_2\cdots-t_nx_n} \,. \tag{4.15}$$

Then, we have the following formula.

Formula 15. The function $S_n(\{x_j\};t)$ is given by

$$\begin{aligned} S_n(\{x_j\};t) \\ &= \frac{1}{x_1(x_1+x_2)(x_1+x_2+x_3)\cdots(x_1+x_2+\cdots+x_n)} \\ &- \frac{e(x_1,t)}{x_1x_2(x_2+x_3)(x_2+x_3+x_4)\cdots(x_2+\cdots+x_n)} \\ &+ \frac{e(x_1+x_2,t)}{(x_1+x_2)x_2x_3(x_3+x_4)(x_3+x_4+x_5)\cdots(x_3+\cdots+x_n)} \\ &- \frac{e(x_1+x_2+x_3,t)}{(x_1+x_2+x_3)(x_2+x_3)x_3x_4(x_4+x_5)(x_4+x_5+x_6)\cdots(x_4+\cdots+x_n)} \\ &+(-1)^n \frac{e(x_1+x_2+\cdots+x_n,t)}{(x_1+x_2+\cdots+x_n)(x_2+\cdots+x_n)(x_3+\cdots+x_n)\cdots(x_{n-1}+x_n)x_n}\,, \end{aligned} \tag{4.16}$$

under the condition that $x_{j_1}+x_{j_2}+\cdots+x_{j_s} \neq 0$ for any set $j_1, j_2, \ldots, j_s$ of $1, 2, \ldots, n$, where $e(x,t)$ is defined by

$$e(x,t) = \mathrm{e}^{-tx} \,. \tag{4.17}$$

For example, we have

$$S_1(x_1;t) = \frac{1-e(x_1,t)}{x_1}\,, \tag{4.18a}$$

$$S_2(x_1,x_2;t) = \frac{1}{x_1(x_1+x_2)} - \frac{e(x_1,t)}{x_1x_2} + \frac{e(x_1+x_2,t)}{(x_1+x_2)x_2}\,, \tag{4.18b}$$

and

$$\begin{aligned} S_3(\{x_j\};t) = {} & \frac{1}{x_1(x_1+x_2)(x_1+x_2+x_3)} - \frac{e(x_1,t)}{x_1x_2(x_2+x_3)} \\ & + \frac{e(x_1+x_2,t)}{(x_1+x_2)x_2x_3} - \frac{e(x_1+x_2+x_3,t)}{(x_1+x_2+x_3)(x_2+x_3)x_3}\,. \end{aligned} \tag{4.18c}$$

The proof of Formula 15 is given by mathematical induction as follows. If we assume Eq. (4.16) for n, then we obtain

$$S_{n+1}(\{x_j\};t) = \int_0^t dt_1 S_n(x_2,x_3,\ldots,x_{n+1};t_1)\,\mathrm{e}^{-t_1x_1} = M_{n+1}(x_1,x_2,\ldots,x_{n+1})$$
$$-\frac{e(x_1,t)}{x_1x_2(x_2+x_3)\cdots(x_2+\cdots+x_{n+1})}+\cdots$$
$$+(-1)^{n+1}\frac{e(x_1+x_2+\cdots+x_{n+1},t)}{(x_1+x_2+\cdots+x_{n+1})(x_2+\cdots+x_{n+1})\cdots x_{n+1}}\,. \tag{4.19}$$

Here, $M_{n+1}(x_1,x_2,\ldots,x_{n+1})$ is defined by

$$M_{n+1}(x_1,x_2,\ldots,x_{n+1})$$
$$=\frac{1}{x_1x_2(x_2+x_3)\cdots(x_2+\cdots+x_{n+1})}$$
$$-\frac{1}{(x_1+x_2)x_2x_3(x_3+x_4)(x_3+x_4+x_5)\cdots(x_3+\cdots+x_{n+1})}$$
$$+\cdots\cdots\cdots$$
$$+(-1)^{n+1}\frac{1}{(x_1+x_2+\cdots+x_{n+1})(x_2+\cdots+x_{n+1})\cdots(x_n+x_{n+1})x_{n+1}}\,. \tag{4.20}$$

Now, we have the following relation.

Formula 16. The function $M_{n+1}(\{x_j\})$ defined by (4.20) is reducible to the following expression:

$$M_{n+1}(\{x_j\}) = \frac{1}{x_1(x_1+x_2)(x_1+x_2+x_3)\cdots(x_1+x_2+\cdots+x_{n+1})}\,. \tag{4.21}$$

This is also easily derived by mathematical induction. Now we put

$$P_n(\{x_j\}) = M_n(\{x_j\}) - \frac{1}{x_1(x_1+x_2)\cdots(x_1+\cdots+x_n)}\,. \tag{4.22}$$

If we assume $P_n(\{x_j\}) = 0$ for any $\{x_j\}$, then we obtain

$$(x_1+x_2+\cdots+x_{n+1})P_{n+1}(\{x_j\})$$
$$= P_n(x_1,x_2,\ldots,x_n) - P_n(x_2,x_3,\ldots,x_{n+1}) = 0\,. \tag{4.23}$$

This yields the proof of Formula 16. Therefore we finally arrive at Formula 15. Using Formula 15, we obtain the following result.

Theorem V. *For any positive integer n, we have*

$$\frac{d^n\mathrm{e}^{tA}}{dA^n} = n!\,\mathrm{e}^{tA}S_n(\{\delta_j\};t)\,, \tag{4.24}$$

where $S_n(\{x_j\};t)$ is given by (4.16) *and $\delta_j \equiv \delta_A^{(j)}$ is defined by* (4.3).

The proof is evident from Formula 13 and Eq. (4.15).

Then, the derivative of A^n is given in the following.

Formula 17. For any positive integer n, we have

$$\frac{d^nA^k}{dA^n} = 0 \quad \text{for } k < n, \qquad \frac{d^nA^n}{dA^n} = n!\,, \tag{4.25a}$$

and

$$\frac{d^nA^k}{dA^n} = n!\left[\frac{d^k}{dt^k}(\mathrm{e}^{tA}S_n(\{\delta_j\};t))\right]_{t=0} \quad \text{for } k > n\,. \tag{4.25b}$$

It will be instructive to give a simple example of Formula 17, namely

$$\frac{d^2A^3}{dA^2} = 2(3A - 2\delta_1 - \delta_2)\,, \tag{4.26a}$$

or equivalently

$$\frac{d^2A^3}{dA^2} : dA \cdot dA = 6AdA \cdot dA - 4(\delta_A \cdot dA) \cdot dA - 2dA \cdot (\delta_A \cdot dA)\,. \tag{4.26b}$$

It should be remarked here that the higher-derivatives are linear, namely we have the following formula.

Formula 18. If $f(A)$ and $g(A)$ are n-times differentiable with respect to A, then we have

$$\frac{d^n}{dA^n}(f(A) + g(A)) = \frac{d^nf(A)}{dA^n} + \frac{d^ng(A)}{dA^n}\,. \tag{4.27}$$

Now we derive the n^{th} derivative of a general operator-valued function $f(A)$. For this purpose, we make use of the inverse Laplace transformation

$$f(x) = \frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty} \hat{f}(s)\mathrm{e}^{sx}ds\,. \tag{4.28}$$

Formally, we have

$$\frac{d^nf(A)}{dA^n} = \frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty} \hat{f}(s)\frac{d^n\mathrm{e}^{sA}}{dA^n}ds = \frac{n!}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty} \hat{f}(s)\mathrm{e}^{sA}S_n(\{\delta_j\};s)\,ds\,. \tag{4.29}$$

From Formula 15, the factor $\mathrm{e}^{sA}S_n(\{\delta_j\};s)$ in (4.29) is rewritten in the form

$$\mathrm{e}^{sA}S_n(\{\delta_j\};s) = \sum_k a_{n,k}(\{\delta_j\})\exp(sA - sb_k(\{\delta_j\})) \tag{4.30}$$

with $b_k = \delta_1 + \delta_2 + \cdots + \delta_k$ and $a_{n,0} = M_n(\{\delta_j\})$,

$$a_{n,k}(\delta_1,\ldots,\delta_n) = -a_{n-1,k-1}(\delta_2,\ldots,\delta_n)/(\delta_1 + \cdots + \delta_k)$$

$$= \frac{(-1)^k}{(\delta_1 + \cdots + \delta_k)(\delta_2 + \cdots + \delta_k)\cdots\delta_k\delta_{k+1}(\delta_{k+1} + \delta_{k+2})\cdots(\delta_{k+1} + \cdots + \delta_n)} \tag{4.31a}$$

for $1 \leqq k \leqq n-1$, and

$$a_{n,n} = \frac{(-1)^n}{(\delta_1 + \cdots + \delta_n)(\delta_2 + \cdots + \delta_n)\cdots(\delta_{n-1}+\delta_n)\delta_n} . \tag{4.31b}$$

Then, using the inverse Laplace transformation, we arrive at the following.

Theorem VI. *If $f(x)$ has a Laplace transform, then we have*

$$\frac{d^n f(A)}{dA^n} = n! \sum_k a_{n,k}(\{\delta_j\}) f(A - b_k(\{\delta_j\})) \tag{4.32}$$

with $a_{n,k}(\{\delta_j\})$ and $b_k(\{\delta_j\})$ given by (4.31a) *and* (4.31b).

For example, we obtain Theorem I for $n = 1$, and the following generalized formulas.

Formula 19. When $f(x)$ has a Laplace transform, we have

$$\frac{d^2 f(A)}{dA^2} = 2!\left[\frac{f(A) - f(A-\delta_1)}{\delta_1\delta_2} - \frac{f(A) - f(A-(\delta_1+\delta_2))}{(\delta_1+\delta_2)\delta_2}\right], \tag{4.33a}$$

and

$$\frac{d^3 f(A)}{dA^3} = 3!\left[\frac{f(A) - f(A-\delta_1)}{\delta_1\delta_2(\delta_2+\delta_3)} - \frac{f(A) - f(A-(\delta_1+\delta_2))}{(\delta_1+\delta_2)\delta_2\delta_3}\right.$$
$$\left. + \frac{f(A) - f(A-(\delta_1+\delta_2+\delta_3))}{(\delta_1+\delta_2+\delta_3)(\delta_2+\delta_3)\delta_3}\right]. \tag{4.33b}$$

These formulas are derived immediately from Eqs. (4.18) and (4.18). Higher-order derivatives for $n \geqq 4$ are also easily obtained from Formula 15.

(ii) Direct method for deriving higher derivatives. It will be instructive to explain here a direct method for deriving successively higher derivatives such as d^2A^n/dA^2 and d^3A^n/dA^3 for a positive integer n, using lower derivatives such as dA^n/dA and d^2A^n/dA^2, respectively.

First we remark here the following general scheme.

Formula 20 (Direct general scheme). When the differential $d^n f(A)$ is given in the form

$$d^n f(A) = \sum_j g_j(A) h_j(\{\delta_k\}) : (dA)^n , \tag{4.34}$$

we have

$$d^{n+1} f(A) = \sum_j \{(dg_j(A))h_j(\{\delta_k\}) + g_j(A) d(h_j\{\delta_k\})\} \cdot (dA)^n) . \tag{4.35}$$

Here, $dh_j(\{\delta_k\})$ can be calculated using the relation

$$d(\delta_A^n \cdot dA) = f_n(\delta_1, \delta_2) : dA \cdot dA \tag{4.36}$$

with $f_1(\delta_1,\delta_2)=0,\ f_2(\delta_1,\delta_2)=\delta_2-\delta_1$ and

$$f_n(\delta_1,\delta_2)=\frac{1}{\delta_1\delta_2}\{(\delta_1^{n+1}-\delta_2^{n+1})-(\delta_1-\delta_2)(\delta_1+\delta_2)^n\}$$

$$=(\delta_2-\delta_1)\sum_{k=1}^{n-1}\left(\binom{n}{k}-1\right)\delta_1^{k-1}\delta_2^{n-k-1}\,. \tag{4.37}$$

The formula (4.35) is evident from the definition of higher differentials. The proof of (4.36) is given by the mathematical induction method as follows. If we assume (4.36) with (4.37), then we obtain

$$d(\delta_A^{n+1})\cdot dA=(d\delta_A)\cdot\delta_A^n(dA)+\delta_A(d(\delta_A^n\cdot dA))\,. \tag{4.38}$$

Here we note that

$$(d\delta_A)\cdot\delta_A^n(dA)=\delta_{dA}\cdot\delta_A^n(dA)=dA\cdot\delta_A^n(dA)-\delta_A^n(dA)\cdot dA$$

$$=(\delta_2^n-\delta_1^n):dA\cdot dA\,, \tag{4.39}$$

and

$$\delta_A(d(\delta_A^n\cdot dA))=f_n(\delta_1,\delta_2)\delta_A(dA\cdot dA)$$

$$=f_n(\delta_1,\delta_2)(A(dA\cdot dA)-(dA\cdot dA)A)$$

$$=f_n(\delta_1,\delta_2)(\delta_1+\delta_2):dA\cdot dA\,, \tag{4.40}$$

using the relation

$$(dA\cdot dA)A=dA\cdot(AdA-\delta_A(dA))$$

$$=A(dA\cdot dA)-\delta_A(dA)\cdot dA-dA\cdot\delta_A(dA)\,. \tag{4.41}$$

Thus, we obtain the recursion equation

$$f_{n+1}(\delta_1,\delta_2)=(\delta_2^n-\delta_1^n)+(\delta_1+\delta_2)f_n(\delta_1,\delta_2) \tag{4.42}$$

with $f_1(\delta_1,\delta_2)=0$. The solution of (4.42) is easily shown to be given by (4.37) for $n+1$.

For example, the derivation d^2A^n is calculated directly from dA^n, using Formula 20 as follows.

We start from formula (3.8), namely

$$dA^n=(A^n-(A-\delta_A)^n)\delta_A^{-1}\cdot dA\,. \tag{4.43}$$

Using Formula 20, we have

$$d^2A^n=\sum_{k=1}^{n}(-1)^{k-1}\binom{n}{j}d(A^{n-k}\delta_A^{k-1})\cdot dA$$

$$=2\left(\frac{A^n-(A-\delta_1)^n}{\delta_1\delta_2}-\frac{A^n-(A-(\delta_1+\delta_2))^n}{(\delta_1+\delta_2)\delta_2}\right):dA\cdot dA\,. \tag{4.44}$$

Here we have used (4.43) and (4.36) to calculate dA^{n-k} and $d\delta_A^{k-1} \cdot dA$ in (4.44). The above formula (4.44) is also obtained from the general formula (4.32), as it should be. Similarly we can calculate d^kA^n and $d^kf(A)$ in this direct method, using the following formula.

Formula 21. For a product $dA \cdot - - - - \cdot dA$ of n elements $\{dA\}$, we have

$$\delta_A : \underbrace{dA \cdot - - - - \cdot dA}_{n} = (\delta_1 + \delta_2 + \cdots + \delta_n) : \underbrace{dA \cdot dA \cdot - - - - \cdot dA}_{n} . \tag{4.45}$$

This is easily derived recursively from the relation

$$\delta_A : dA \cdot dA \cdot - - - - \cdot dA = (\delta_A dA) \cdot dA \cdot - - - - \cdot dA + dA \cdot \delta_A(dA \cdot - - - - \cdot dA) . \tag{4.46}$$

In fact, the higher-derivative $d^nf(A)/dA^n$ can be derived formally using the above direct method as follows. Now we start with Theorem I, namely

$$\delta_A(df(A)) = \delta_{f(A)} \cdot dA . \tag{4.47}$$

Differentiating both sides of (4.47), we obtain

$$\delta_{dA}(df(A)) + \delta_A(d^2f(A)) = \delta_{df(A)} \cdot dA = -\delta_{dA}(df(A)) . \tag{4.48}$$

Here we have used the relations that $d(\delta_A Q) = \delta_{dA}Q + \delta_A(dQ)$ and $d^2A = 0$. Thus, we arrive at the relation

$$\delta_A(d^2f(A)) = -2\delta_{dA}(df(A)) = 2\delta_{df(A)} \cdot dA . \tag{4.49}$$

Differentiating both sides of (4.49) again, we obtain

$$\delta_A(d^3f(A)) = 3\delta_{d^2f(A)} \cdot dA . \tag{4.50}$$

By mathematical induction, we obtain the following.

Theorem VII. *When $f(x)$ is analytic for $|x - a| < b$, the n^{th} differential $d^nf(A)$ satisfies the following recursive relation*:

$$\delta_A(d^nf(A)) = n\delta_{d^{n-1}f(A)} \cdot dA \tag{4.51}$$

in the domain $\mathscr{D}$ defined by (3.11). *More explicitly, $d^nf(A) = n!(-\delta_A^{-1}\delta_{dA})^n f(A)$, namely*

$$(\delta_1 + \cdots + \delta_n)\frac{d^nf(A)}{dA^n} : (dA)^n = n\left[\frac{d^{n-1}f(A)}{dA^{n-1}} : (dA)^{n-1}, dA\right] , \tag{4.52}$$

or equivalently

$$(\delta_1 + \cdots + \delta_n) f_n(A, \delta_1, \ldots, \delta_n) = n(f_{n-1}(A, \delta_1, \ldots, \delta_{n-1}) - f_{n-1}(A - \delta_1, \delta_2, \ldots, \delta_n)) \tag{4.53}$$

for $f_n(A, \delta_1, \ldots, \delta_n) \equiv d^n f(A)/dA^n$.

Equation (4.53) in Theorem VII is derived using the following formula.

Formula 22. When $f(x, y_1, \ldots, y_{n-1})$ is a convergent power series of x and $\{y_j\}$, the following relation holds:

$$dA \cdot f(A, \delta_1, \ldots, \delta_{n-1}) : (dA)^{n-1} = f(A - \delta_1, \delta_2, \ldots, \delta_n) : (dA)^n . \tag{4.54}$$

This formula is easily derived from the following relation:

$$\begin{aligned} dA \cdot A^m &= A^m \cdot dA - \delta_{A^m} \cdot dA \\ &= A^m \cdot dA - (A^m - (A - \delta_1)^m) \cdot dA = (A - \delta_1)^m \cdot dA \end{aligned} \tag{4.55}$$

for any positive integer m.

Note that the right-hand side of (4.53) contains the factor $(\delta_1 + \cdots + \delta_n)$, as is easily seen recursively. Then, it can be divided by hyperoperator $(\delta_1 + \cdots + \delta_n)$. Thus, we arrive at the following convenient recursive formula on higher-derivatives.

Formula 23. The n^{th} derivative $f_n(A, \delta_1, \ldots, \delta_n)$ is given by the following recursive formula:

$$f_1(A, \delta_1) = \frac{f(A) - f(A - \delta_1)}{\delta_1} = \int_0^1 dt f^{(1)}(A - t\delta_1) , \tag{4.56}$$

and

$$f_{n+1}(A, \delta_1, \ldots, \delta_{n+1}) = \frac{n+1}{\delta_{n+1}} (f_n(A, \delta_1, \ldots, \delta_n) - f_n(A, \delta_1, \ldots, \delta_{n-1}, \delta_n + \delta_{n+1})) . \tag{4.57}$$

This is easily derived from Theorem VII, using Formula 16. This recursive formula gives again the explicit higher-derivatives (4.32) and Formula 19, as is easily confirmed.

(iii) Higher derivatives of hyperoperators. Here we introduce a derivation of the hyperoperator $f(\delta_A)$ as follows.

Formula 24. We have

$$df(\delta_A) \cdot dA = \left(\frac{f(\delta_1) - f(\delta_1 + \delta_2)}{\delta_2} - \frac{f(\delta_2) - f(\delta_1 + \delta_2)}{\delta_1} \right) : dA \cdot dA . \tag{4.58}$$

The validity of this formula is easily confirmed from Eq. (4.36) with (4.37). Similarly, we can define the derivation of any hyperoperator of the form $f(A, \delta_1, \ldots, \delta_n)$.

Using these derivatives of hyperoperators, we can derive again formula (4.31) and Formula 19.

(iv) Operator Taylor expansion. Using the above higher-derivatives $d^n f(A)/dA^n$, we obtain the following Taylor expansion.

Theorem VIII (Operator expansion theorem). *When $f(x)$ is analytic for $|x-a|<b$, $f(A+xB)$ is expanded as*

$$f(A+xB)=\sum_{n=0}^{\infty}\frac{x^n}{n!}\frac{d^n f(A)}{dA^n}:B^n=\sum_{n=0}^{\infty}(-x\,\delta_A^{-1}\delta_B)^n f(A)$$

$$=f(A)+\sum_{n=1}^{\infty}x^n\int_0^1 dt_1\int_0^{t_1}dt_2\cdots\int_0^{t_{n-1}}dt_n f^{(n)}(A-t_1\delta_1-\cdots-t_n\delta_n):B^n \tag{4.59}$$

in the domain $\mathscr{D}$ defined by (3.11). Here, $f^{(n)}(x)$ denotes the n^{th} derivative of $f(x)$.

The above operator expansion (4.59) is also formally obtained from the resolvent expansion formula (4.9) as follows:

$$\frac{d^n f(A)}{dA^n}:B^n=\frac{n!}{2\pi i}\int_C\frac{f(z)}{z-A}\left(B\frac{1}{z-A}\right)^n dz$$

$$=\frac{n!}{2\pi i}\int_C\frac{f(z)}{(z-A)(z-A+\delta_1)\cdots(z-A+\delta_1+\cdots+\delta_n)}dz:B^n\,. \tag{4.60}$$

Here we have used the commutation relations

$$B\frac{1}{z-A}=\frac{1}{z-A+\delta_A}\cdot B=\frac{1}{z-A+\delta_1}\cdot B\,,$$

$$\left(B\frac{1}{z-A}\right)^2=\left(\frac{1}{z-A+\delta_A}\cdot B\right)\left(\frac{1}{z-A+\delta_A}\cdot B\right)$$

$$=\frac{1}{(z-A+\delta_1)(z-A+\delta_1+\delta_2)}:B\cdot B\,, \tag{4.61}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$\left(B\frac{1}{z-A}\right)^n=\frac{1}{(z-A+\delta_1)(z-A+\delta_1+\delta_2)\cdots(z-A+\delta_1+\cdots+\delta_n)}:B^n\,.$$

Thus, we arrive at the formula

$$\frac{d^n f(A)}{dA^n}=\frac{n!}{2\pi i}\int_C\frac{f(z)}{(z-A)(z-A+\delta_1)\cdots(z-A+\delta_1+\cdots\delta_n)}\,. \tag{4.62}$$

By mathematical induction, we can derive (4.59) from the above formula (4.62). Although this derivation is much simpler, the previous elementary derivation using the Feynman formula is more transparent for understanding the structure of higher-order derivatives, as already shown.

(v) Higher derivations with respect to a parameter. The above formulas can be applied to an operator-valued function $f(A(t))$ of $A(t)$ with a parameter t. It is easy to derive the following theorem.

Theorem IX. *If $f(A)$ and $A(t)$ are n-times differentiable with respect to A and t, respectively, then we have*

$$\frac{d^2 f(A(t))}{dt^2} = \frac{d^2 f(A(t))}{dA(t)^2} : \frac{dA(t)}{dt} \cdot \frac{dA(t)}{dt} + \frac{df(A(t))}{dA(t)} \cdot \frac{d^2 A(t)}{dt^2},$$

$$\begin{aligned}\frac{d^3 f(A(t))}{dt^3} &= \frac{d^3 (A(t))}{dA(t)^3} : \frac{dA(t)}{dt} \cdot \frac{dA(t)}{dt} \cdot \frac{dA(t)}{dt} \\ &\quad + 2\frac{d^2 f(A(t))}{dA(t)^2} : \frac{dA(t)}{dt} \cdot \frac{d^2 A(t)}{dt^2} + \frac{d^2 fA(t)}{dA(t)^2} : \frac{d^2 A(t)}{dt^2} \cdot \frac{dA(t)}{dt} \\ &\quad + \frac{df(A(t))}{dA(t)} \cdot \frac{d^3 A(t)}{dt^3}. \end{aligned} \tag{4.63}$$

For a general positive integer n, we have the following recursive formula. If we put

$$\begin{aligned}\frac{d^n f(A(t))}{dt^n} &= \sum_{s=1}^{n} \sum_{\{k_j \geqq 1\}} c_n(k_1, k_2, \ldots, k_s) \\ &\quad \times \frac{d^s f(A(t))}{dA(t)^s} : \frac{d^{k_1} A(t)}{dt^{k_1}} \cdot \frac{d^{k_2} A(t)}{dt^{k_2}} \cdot \cdots \cdot \frac{d^{k_s} A(t)}{dt^{k_s}} \end{aligned} \tag{4.64}$$

with $k_1 + k_2 + \cdots + k_s = n$, then we have

$$\begin{aligned}\frac{d^{n+1} f(A(t))}{dt^{n+1}} &= \sum_{s=1}^{n} \sum_{\{k_j \geqq 1\}} c_n(k_1, k_2, \ldots, k_s) \\ &\quad \times \frac{d^{s+1} f(A(t))}{dA(t)^{s+1}} : \frac{dA(t)}{dt} \cdot \frac{d^{k_1} A(t)}{dt^{k_1}} \cdot \cdots \cdot \frac{d^{k_s} A(t)}{dt^{k_s}} \\ &\quad + \sum_{s=1}^{n} \sum_{j=1}^{s} \sum_{\{k_j \geqq 1\}} c_n(k_1, k_2, \ldots, k_s) \\ &\quad \times \frac{d^s f(A(t))}{dA(t)^s} : \frac{d^{k_1} A(t)}{dt^{k_1}} \cdot \cdots \cdot \frac{d^{k_j+1} A(t)}{dt^{k_j+1}} \cdot \cdots \cdot \frac{d^{k_s} A(t)}{dt^{k_s}}. \end{aligned} \tag{4.65}$$

When all the quantities $A(t), A^{(1)}(t), \ldots,$ and $A^{(n)}(t)$ commute with each other, these formulas reduce to Bell's polynomials concerning ordinary derivatives. They will be useful in practical applications.

V. Partial Differentiation for Multivariate Functions

In the present section, we discuss partial derivatives of an operator-valued function of several variables, for example, $f(A,B)$. The derivation $df(A,B)$ is defined as

$$df(A,B) = \lim_{h\to 0} \frac{f(A+hdA, B+hdB) - f(A,B)}{h}. \tag{5.1}$$

The differential of $f(\{A_j\})$ is defined similarly as

$$df(\{A_j\}) = \lim_{h\to 0} \frac{1}{h}[f(\{A_j + hdA_j\}) - f(\{A_j\})]. \tag{5.2}$$

Then the partial derivative $\partial f(\{A_j\})/\partial A_k$ is defined in

$$df(\{A_j\}) = \sum_k \frac{\partial f(\{A_j\})}{\partial A_k} \cdot dA_k. \tag{5.3}$$

The partial derivative $\partial f/\partial A_k$ is a hyperoperator which maps the operator dA_k to the derivation for $dA_j \equiv 0 (j \neq k)$ and which is expressed in terms of $\{A_j\}$ and $\{\delta_{A_j}\}$. We have the following.

Theorem X. *If there exist the partial derivatives* $\{\partial f(\{A_j\})/\partial A_k\}$ *for all k, then we have*

$$\frac{d}{dt} f(\{A_j(t)\}) = \sum_k \frac{\partial f(\{A_j(t)\})}{\partial A_k(t)} \cdot \frac{dA_k(t)}{dt}. \tag{5.4}$$

The proof is quite similar to that of Theorem II.

Now we have the following formula.

Formula 25. If $f(A,B)$ and $g(A,B)$ are partially differentiable with respect to both A and B, then we have

$$\frac{\partial}{\partial A}(f(A,B)g(A,B)) = f(A,B)\frac{\partial g(A,B)}{\partial A} + (g(A,B) - \delta_{g(A,B)})\frac{\partial f(A,B)}{\partial A}, \tag{5.5}$$

and a similar formula holds for the partial derivative with respect to B.

The proof is given as follows:

$$\begin{aligned}\frac{\partial}{\partial A}(f(A,B)g(A,B)) \cdot dA &= \lim_{h\to 0} \frac{f(A+hdA,B)g(A+hdA,B) - f(A,B)g(A,B)}{h} \\ &= \left(\frac{\partial f}{\partial A} \cdot dA\right) g + f\frac{\partial g}{\partial A} \cdot dA \\ &= \left(f\frac{\partial g}{\partial A} + (g - \delta_g)\frac{\partial f}{\partial A}\right) \cdot dA, \end{aligned} \tag{5.6}$$

namely

$$\frac{\partial}{\partial A}(fg) = f\frac{\partial g}{\partial A} + (g - \delta_g)\frac{\partial f}{\partial A}. \tag{5.7}$$

Now we introduce a tilde hyperoperator $\tilde{f}$ of any operator f as

$$A_{\tilde{j}} \equiv \tilde{A}_j = A_j - \delta_{A_j}, \qquad (fg)\tilde{} = \tilde{g}\tilde{f}, \qquad (cf)\tilde{} = c\tilde{f}, \qquad (f+g)\tilde{} = \tilde{f} + \tilde{g} \tag{5.8}$$

for any number c and any operators f and g. Then, we can easily derive the following formulas on the tilde hyperoperator $\tilde{f}$.

Formula 26. When $f \equiv f(\{A_j\})$ is a convergent noncommutative power series of $\{A_j\}$, we have

$$Qf = (\tilde{f}Q) \equiv \tilde{f}(Q) \tag{5.9}$$

for any operator Q.

The proof is easily given using the rule (5.8) by extending the procedure (4.55).

Formula 27. When $f(\{A_j\})$ and $g(\{A_j\})$ are convergent noncommutative power series of $\{A_j\}$, we have the following commutation relation:

$$f\tilde{g}(Q) = \tilde{g}(fQ) \tag{5.10}$$

for any operator Q.

The proof is given as

$$f\tilde{g}(Q) = fQ_g = (fQ)g = \tilde{g}(fQ) \tag{5.11}$$

for any operator Q, using Formula 26.

Furthermore, we have the following relation.

Formula 28. When $f \equiv f(\{A_j\})$ is a convergent noncommutative power series of $\{A_j\}$, we have

$$\delta_f = f - \tilde{f}\,. \tag{5.12}$$

This expression is immediately obtained from Formula 26 and is an extension of Formula 4. Now we may regard the expression $\tilde{f} = f - \delta_f$ as a definition of $\tilde{f}$ instead of the construction rule (5.8).

In general, we have the following formula concerning the multiproduct $f_1(\{A_j\}) \cdots f_n(\{A_j\})$.

Formula 29. If $\{f_j(\{A_k\})\}$ are partially differentiable with respect to A_k, then we have

$$\frac{\partial}{\partial A_k}(f_1 f_2 \cdots f_n) = \sum_{j=1}^{n} f_1 f_2 \cdots f_{j-1} \tilde{f}_n \tilde{f}_{n-1} \cdots \tilde{f}_{j+1} \left(\frac{\partial f_j}{\partial A_k}\right)\,. \tag{5.13}$$

The derivation of Formula 29 is easily given by using Formula 26. The order of the operator functions is crucial in (5.13).

We have also the following formula.

Formula 30. If $f(\{A_j\})$, $g(\{A_j\})$ and $h(\{A_j\})$ are partially differentiable, then we have

$$\frac{\partial}{\partial A_k} f(g(\{A_j\}), h(\{A_j\})) = \frac{\partial f}{\partial g}\frac{\partial g}{\partial A_k} + \frac{\partial f}{\partial h}\frac{\partial h}{\partial A_k}\,. \tag{5.14}$$

This is easily derived as in Theorem III.

It is also interesting to remark the following theorem.

Theorem XI. *If $f(\{A_j\})$ is partially differentiable with respect to all $\{A_j\}$, then we have*

$$\delta_{f(\{A_j\})} = \sum_k \frac{\partial f(\{A_j\})}{\partial A_k}\delta_{A_k} \,. \tag{5.15}$$

The proof is given using the mathematical induction method as follows. We assume that

$$\delta_{f_n(\{A_j\})} = \sum_k \frac{\partial f_n(\{A_j\})}{\partial A_k}\delta_{A_k} \tag{5.16}$$

for any polynomial $f_n(\{A_j\})$ of order n. Now, similarly to Formula 1 we note first that

$$\delta_{f(\{A_j\})g(\{A_j\})} = f(\{A_j\})\delta_{g(\{A_j\})} + g(\{A_j\})\delta_{f(\{A_j\})} - \delta_{g(\{A_j\})}\delta_{f(\{A_j\})} \,. \tag{5.17}$$

Then, using assumption (5.16) we obtain

$$\begin{aligned}
\delta_{A_k f_n(\{A_j\})} &= A_k\delta_{f_n(\{A_j\})} + f_n(\{A_j\})\delta_{A_k} - \delta_{f_n(\{A_j\})}\delta_{A_k} \\
&= A_k \sum_j \frac{\partial f_n}{\partial A_j}\delta_{A_j} + f_n\delta_{A_k} - \delta_{f_n}\delta_{A_k} \\
&= \left(A_k\frac{\partial f_n}{\partial A_k} + f_n - \delta_{f_n}\right)\delta_{A_k} + A_k\sum_{j\neq k}\frac{\partial f_n}{\partial A_j}\delta_{A_j} \\
&= \frac{\partial(A_k f_n)}{\partial A_k}\delta_{A_k} + \sum_{j\neq k}\frac{\partial(A_k f_n)}{\partial A_j}\delta_{A_j} \\
&= \sum_j \frac{\partial(A_k f_n(\{A_j\}))}{\partial A_j}\partial_{A_j}
\end{aligned} \tag{5.18}$$

for any k, where $f_n = f_n(\{A_j\})$. Thus, we arrive at the relation

$$\delta_{f_{n+1}(\{A_j\})} = \sum_k \frac{\delta f_{n+1}(\{A_j\})}{\partial A_k}\delta_{A_k} \,. \tag{5.19}$$

Therefore, we obtain formula (5.15) for any operator-valued function $f(\{A_j\})$ that can be expressed in a non-commuting power series of the operator polynomials $\{f_n(\{A_j\})\}$.

Now we consider explicitly the partial derivative of $f(\{A_j\})$.

Formula 31. When $f(\{A_j\})$ is expressed as a convergent noncommutative power series of $\{A_j\}$, namely

$$f(\{A_j\}) = \sum_{\{t_{jk}\}} a(\{t_{jk}\})A_1^{t_{11}}A_2^{t_{12}}\cdots A_n^{t_{1n}}A_1^{t_{21}}\cdots A_k^{t_{jk}}\cdots \,, \tag{5.20}$$

we have

$$\frac{\partial f}{\partial A_k} = \sum_{\{t_{jk}\}}\sum_j a(\{t_{jk}\})A_1^{t_{11}}\cdots A_k^{t_{jk-1}}(A_{k+1}^{t_{jk+1}}\cdots)\tilde{}\left(\frac{d}{dA_k}A_k^{t_{jk}}\right) \,. \tag{5.21}$$

This formula is easily confirmed using Formulas 26 or 29.

In order to obtain a more convenient formal expression of partial derivatives, we introduce here the following partial inner derivation:

$$\delta_{f(\{A_j\});k}Q = -\delta_{Q;k}f(\{A_j\})\,. \tag{5.22}$$

Here, $\delta_{Q,k}$ denotes taking the commutation relation only with respect to the operator A_k. For example,

$$\delta_{Q;k}\cdot(A_kA_jA_k^2) = [Q,A_k]A_jA_k^2 + A_kA_j[Q,A_k^2] \tag{5.23}$$

for $j \neq k$. Using this partial inner derivation, we find the following formula.

Formula 32.

$$\frac{\partial f(\{A_j\})}{\partial A_k} = \delta_{f(\{A_j\});k}\delta_{A_k}^{-1}\,. \tag{5.24}$$

In order to formulate higher derivatives of $f(\{A_j\})$, we introduce here an ordered partial inner derivation $\hat{\partial}_{B_j,B_k,\ldots,B_m;A_j,A_k,\ldots,A_m}$ which is a linear hyperoperator to map any operator of the form $f_1(A_{j1})f_2(A_{j2})\cdots f_n(A_{j_n})$ as

$$\begin{aligned}
&\hat{\partial}_{B_j,B_k,\ldots,B_m;A_j,A_k,\ldots,A_m}f_1(A_{j1})f_2(A_{j2})\cdots f_n(A_{jn}) \\
&= \sum \sum_{k_1\leqq k_2\leqq\cdots\leqq k_m} \cdots \sum f_1(A_{j1})\cdots[B_j,f_{k1}(A_j)]\delta(j_{k_1},j)\cdots \\
&\quad \cdots[B_k,f_{k_2}(A_k)]\delta(j_{k_2},k)\cdots[B_m,f_{k_m}(A_m)]\delta(j_{k_m},m)\cdots f_n(A_{j_n})\,.
\end{aligned} \tag{5.25}$$

For example,

$$\begin{aligned}
\hat{\partial}_{B_1,B_2;A_1,A_2}(A_1^pA_2^qA_1^rA_2^s) &= A_1^pA_2^q[A_1^r,B_1][A_2^s,B_2] + [A_1^p,B_1]A_2^qA_1^r[A_2^s,B_2] \\
&\quad + [A_1^p,B_1][A_2^q,B_2]A_1^rA_2^s\,.
\end{aligned} \tag{5.26}$$

Here, $\delta(j,k)$ denotes the Kronecker delta function. Using this ordered partial inner derivation, the n^{th} order differential

$$d_{j_1,j_2,\ldots,j_n}f(\{A_j\}) \equiv f^{(n)}_{j_1,j_2,\ldots,j_n}(\{A_j\},\{\partial_{ij}\}) : dA_{j_1}\cdots dA_{j_2}\cdot\text{-}\text{-}\text{-}\text{-}\cdot dA_{j_n}\,, \tag{5.27}$$

is defined by

$$d_{j_1,j_2,\ldots,j_n} = \partial_{\delta_{A_{j_1}}^{-1}dA_{j_1},\ldots,\delta_{A_{j_n}}^{-1}dA_{j_n};A_{j_1},\ldots,A_{j_n}}\,. \tag{5.28}$$

Here, we have assumed that the set $(j_1,j_2,\ldots,j_n)$ contains the figures $1,2,\ldots,q$, n_1 times, n_2 times, $\ldots n_q$ times, respectively. Now, we have the following operator Taylor expansion formula:

Formula 33.

$$\begin{aligned}
f(\{A_j + xB_j\}) &= \sum_{n=0}^{\infty} x^n \sum_{j_1,\ldots,j_n} \\
&\quad \times f^{(n)}_{j_1,j_2,\ldots,j_n}(\{A_j\},\{\partial_{ij}\}) : B_{j_1}\cdot\text{-}\text{-}\text{-}\text{-}\cdot B_{j_n}\,,
\end{aligned} \tag{5.29}$$

where the hyperoperators $\{\partial_{ij}\}$ are defined by

$$\partial_{ij} : B_{j_1}\cdot\text{-}\text{-}\text{-}\text{-}\cdot B_{j_n} = B_{j_1}\cdot\text{-}\text{-}\text{-}\text{-}\cdot(-\delta_{A_j}B_{j_i})\cdot\text{-}\text{-}\text{-}\text{-}\cdot B_{j_n}\,. \tag{5.30}$$

The hyperoperators ∂_{ij} and ∂_{kl} commute with each other for $k \neq i$. The above formula (5.29) is an extension of Eq. (4.59), namely

$$f(A+xB) = \sum_{n=0}^{\infty} x^n(-\delta_A^{-1}\delta_B)^n f(A). \tag{5.31}$$

VI. Operator Integral and Differential Equation

(i) Integral. It is convenient to define an integral of $f(A)$ with respect to A as

$$\int_C f(A)\cdot dA = \int_{A(t_0)}^{A(t)} f(A)\cdot dA = \int_{t_0}^{t_1} f(A(t))\cdot \frac{dA(t)}{dt}\,dt. \tag{6.1}$$

Here, the notation $\int_C$ denotes an integration along the path from $A(t_0)$ to $A(t_1)$ with some appropriate parameter t. In many cases, $f(A)$ may be a hyperoperator which maps $dA(t)/dt$ to another operator.

For example, we have

$$\int \mathrm{e}^{-A}\Delta(A)\cdot dA = -\mathrm{e}^{-A} + \text{constant}, \tag{6.2}$$

which corresponds to an indefinite integral in the ordinary function space. In general, we have the following.

Theorem XII. *When $f(x)$ is analytic for $|x-a|<b$, then we have*

$$\int \frac{\delta_f(A)}{\delta_A}\cdot dA = \int \frac{df(A)}{dA}\cdot dA = f(A) + \text{constant}. \tag{6.3}$$

This is easily seen from Theorem I.

(ii) Operator equations and differential operator-equations. We consider here the following type of operator equation:

$$f(X(t),\{A_j(t)\}) = 0. \tag{6.4}$$

It is not easy to solve for $X(t)$, because of the noncommutativity of $X(t)$ and $\{A_j(t)\}$. Thus, we propose here a new method based on the quantum analysis. First we differentiate (6.4) to get

$$\frac{\partial f}{\partial X(t)}\cdot\frac{dX(t)}{dt} + \sum_j \frac{\partial f}{\partial A_j(t)}\cdot\frac{dA_j(t)}{dt} = 0. \tag{6.5}$$

Then, we obtain

$$\frac{dX(t)}{dt} = -\left(\frac{\partial f}{\partial X(t)}\right)^{-1} \sum_j \frac{\partial f}{\partial A_j(t)}\cdot\frac{dA_j(t)}{dt}. \tag{6.6}$$

This nonlinear differential equation is convenient to solve perturbationally for $X(t)$.

(iii) Exact differential operator-equations. Similarly to an ordinary total differential equation, we consider the following total differential operator-equation:

$$df(\{A_j\}) = 0. \tag{6.7}$$

Then, the solution of (6.7) is given by $f(\{A_j\})=\text{constant}$. Noting that $dAdB \neq dBdA$, we obtain the following.

Theorem XIII. *A differential operator-equation of the form*

$$\sum_{k=1}^{n} f_k(\{A_j\}) \cdot dA_k = 0 \tag{6.8}$$

is an exact differential equation of the form (6.7), *if and only if*

$$\frac{\partial}{\partial A_j}(f_k \cdot dA_k) \cdot dA_j = \frac{\partial}{\partial A_k}(f_j \cdot dA_j) \cdot dA_k \tag{6.9}$$

for all j and k. The general solution of (6.17) *is given by*

$$\sum_{k=1}^{n} \int_{A_k(0)}^{A_k} f_k(A_1,\ldots,A_k,A_{k+1}(0),\ldots,A_n(0)) \cdot dA_k = c \tag{6.10}$$

with some constant c and constant operators $\{A_j(0)\}$.

When the above condition (6.9) is not satisfied, an integrating factor may be multiplied to (6.8) in order to reduce it possibly to an exact differential operator-equation of the form (6.7).

VII. Concluding Remarks

The convergence proof of the formulas in the present paper for unbounded operators can be studied using the strong norm convergence. For example, we have to show

$$\lim_{h\to 0} \left\| \left(\frac{f(A)+hd(A)-f(A)}{h} - \frac{df(A)}{dA} \cdot dA \right) \psi \right\| = 0 \tag{7.1}$$

for $\psi \in \mathscr{D}$ with some appropriate domain $\mathscr{D}$ in a Hilbert space. However, this kind of proof is too mathematical to discuss here. Some preliminary convergence proofs on higher-order exponential product formulas for unbounded operators have been reported by the present author [17].

The quantum analysis will be useful for studying exponential product formulas [8–14,16], the nonequilibrium statistical operator [18–20] and the geometry of canonical correlations on the state space of a quantum system [15].

Acknowledgements. The author would like to thank Professor H. Araki, Professor K. Aomoto, Professor H. Hiai, Professor N. Obata and Dr. R.I. McLachlan for useful comments.

Added in proof. Recently it has been proven that the quantum derivatives $\{d^n f(A)/dA^n\}$ are invariant for any choice of definitions of the differential $df(A)$ satisfying the Leibniz rule and the linearity (M. Suzuki, J. Math. Phys.).

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Communicated by H. Araki