ITERATED COMMUTATORS AND FUNCTIONS OF OPERATORS

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Cleveland, Ohio
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ABSTRACT

A new method is developed by which certain functions of the noncommuting operators A and B can be expressed in a systematic and efficient way in terms of successively higher commutators of the operators. The procedure is designed primarily for polynomials, exponential functions, and analytic functions of the operator (A + B). The method is related to the ordered-operator calculus of Feynman. Certain commutation properties of the operators A and B are represented by polynomials in A and B called iterated commutators. The functions are converted into equivalent forms involving the iterated commutators. All iterated commutators of degree (j + 1) in A and B are combined in a suitable sum to form a new operator $G_{(j)}$. By working only with the $G_{(j)}$ and their commutators, the calculations are simplified and the results are given in an extremely compact notation.
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SUMMARY

Certain commutation properties of two operators A and B are represented by polynomials in A and B called iterated commutators. A method is developed for systematically expressing functions of A and B in terms of the iterated commutators. The method is related to the ordered-operator calculus of Feynman. Compact expressions result because all iterated commutators of the same degree always appear in the same linear combination. The procedure is designed primarily for polynomials, exponential functions, and analytic functions of the operator (A + B). Applications to the important case of exponential functions are given.

INTRODUCTION

Functions of noncommuting operators have been studied extensively over the years, usually within the context of problems arising in mathematics and quantum physics. A survey of results, along with numerous references, has been given recently by Wilcox (ref. 1). One approach in working with such a function is to express it as an expansion in successively higher commutators of the operators involved. The purpose of this report is to present a new method by which explicit forms of the desired type can be developed in a systematic and efficient way for certain functions of interest.

This method is related to the ordered-operator calculus of Feynman (ref. 2). In Feyman's operator calculus, an ordering parameter indicates the sequence in which noncommuting quantities appearing in any product are to be taken. An operator A, which does not otherwise depend on the ordering parameter s, may be written $A_s$, with the ordering index attached as a subscript. Then it is understood that the form of $A_s$ does not depend on s, but its order of operation does and is defined by the convention: The operator with smallest index operates first, and so forth. Thus, $A_s B_s'$ equals BA when $s' > s$, equals AB when $s > s'$, and is undefined when $s = s'$. In the more general case of an operator that is a function of the time, the convention is that time is the
ordering parameter. We can use the notation $A(s)$ to include either case.

With the ordering parameter convention, any functional of the operator functions $A(s)$, $B(s)$, $\ldots$ has a unique interpretation, because the order of operations in any situation is automatically specified by the parameter values. In manipulating such a functional, the algebra and calculus of ordinary numbers may be applied, as though $A(s)$, $B(s)$, $\ldots$ were ordinary commuting functions. "Disentangling" is the name given by Feynman to the process of finding an operator expression for the functional in the usual positional notation, where the order of operation is represented by the position in which the operators are written. Simple examples of disentangling are the following:

$$\exp(A_{1} + B_{0}) = \exp(A) \exp(B)$$

(1)

$$\exp \left( \int_{0}^{1} A_{s} \, ds \right) \exp \left( \int_{0}^{1} B_{s} \, ds \right) = \exp \left( \int_{0}^{1} (A_{s} + B_{s}) \, ds \right) = \exp(A + B)$$

(2)

An example of a full functional is the well-known Dyson formula for the Neumann-Liouville expansion of the unitary time development transformation. The transformation is an exponential functional of a time-dependent Hamiltonian operator function. The ordering is usually exhibited explicitly by the chronological operator, which may be omitted when the Feynman notation is adopted.

The Feynman formalism permits all the results of ordinary analysis to be used in handling operator functionals. However, no general procedure for disentangling functionals is available. Moreover, there does not appear to be any direct way of exploiting any simple commutation properties that the operators may happen to possess. The method presented here deals with this second aspect. Certain commutation properties of two operators $A$ and $B$ are represented by polynomials in $A$ and $B$ called iterated commutators. The procedure given converts polynomials, exponential functions, and analytic functions of $(A + B)$ into equivalent forms in terms of the iterated commutators. All iterated commutators of degree $(j + 1)$ in $A$ and $B$ are combined in a suitable sum to form a new operator $G_{(j)}$. By working only with the $G_{(j)}$ and their commutators, the calculations are simplified and the results can be given in an extremely compact notation.

In the next section, the iterated commutators are defined and their relevant properties are given. In the section EXPANSION IN ITERATED COMMUTATORS, relations are developed that convert a suitable function of two operators into the desired form. Applications to the important case of exponential operators are given in the section EXPONENTIAL FUNCTIONS. As the derivations required are generally quite straightforward, complete details are given only where deemed necessary and a suitable method is indicated in all other cases.
SYMBOLS

A operator
A_s operator with ordering index s
A(s) operator which may depend on ordering parameter s
B operator
C operator in eq. (29)
C(i) operator in Zassenhaus formula
E(i) operator in expansion of C
F(x) analytic function of x
G(j) linear combination of iterated commutators
H operator in BCH formula
H(i) operator in expansion of H
H_0 A + B
P F[λ(A + B)]^{-1} F[λ(A_1 + B_0)]
P_i operator in expansion of P
R F[λ(A + B)] - F[λ(A_1 + B_0)]
s ordering parameter
{(A^n, (B))} [A, . . . [A, [A, B]] . . . ], n commutations
{(A), (B)^n} ... [[A, B], B] . . . , B, n commutations
{(A)^m, (B)^n} \_L \{(A)^m, (B)\}, (B)^{n-1}\}
{(A)^m, (B)^n} \_R \{(A)^{m-1}, (\{(A), (B)^n\})\}

Superscript:
† Hermitian adjoint

ITERATED COMMUTATORS

The simple iterated commutator is

\{(A^n, (B))\} = [A, . . . [A, [A, B]] . . . ] \tag{3}
which defines a linear operation on $B$ obtained by $n$ successive commutations with the operator $A$. The form of equation (3) is a polynomial whose terms each have $n$ factors of $A$ and one of $B$. Similarly,

$$\{(A), (B)^n\} = [\ldots [A, B], B, \ldots, B]$$ (4)

The case $n = 0$ is specified by

$$\{(A)^0, (B)\} = B, \quad \{(A), (B)^0\} = A$$

It is seen that

$$\{(B)^n, (A)\} = (-1)^n \{(A), (B)^n\}$$ (5)

Clearly, the iterated commutators (eqs. (3) and (4)) arise when two operators, one of which is raised to a power, are transposed. The following four theorems are established by induction:

$$\{(A)^n, (B)\} = \sum_{r=0}^{n} (-1)^r \binom{n}{r} A^{n-r} BA^r$$ (6)

$$[A^n, B] = \sum_{r=1}^{n} \binom{n}{r} \{(A)^r, (B)\} A^{n-r}$$ (7a)

$$[A, B^n] = \sum_{r=1}^{n} \binom{n}{r} B^{n-r} \{(A), (B)^r\}$$ (7b)

$$\{(A)^n, (BC)\} = \sum_{r=0}^{n} \binom{n}{r} \{(A)^{n-r}, (B)\} \{(A)^r, (C)\}$$ (8)

A familiar example in which these iterated commutators occur is the Lie expansion, which is the power series

$$\exp(\lambda A) B \exp(-\lambda A) = \sum_{r=0}^{\infty} \left(\frac{\lambda^r}{r!}\right) \{(A)^r, (B)\}$$
There is no unique way to prescribe a commutator \( \{ (A)^m, (B)^n \} \) that reduces to the forms in equations (3) and (4) for the special cases \( n = 1 \) and \( m = 1 \), respectively. Various generalizations suggest themselves. The extended definition of iterated commutator is chosen to be

\[
\{ (A)^m, (B)^n \}_L = \{( (A)^m, (B) ) \}, (B)^{n-1} \}
\]

In the "L-type" of extended commutator (eq. (9)), the simple commutator (eq. (3)) with the \( m \)-fold iteration of the operator \( A \) (the operator appearing in the left-hand position) is formed first, followed by the remaining \((n-1)\) iterations of the other operator, \( B \). An R-type commutator, for which the prescription is reversed, is easily seen from equation (5) to satisfy the relation

\[
\{ (A)^m, (B)^n \}_R = (-1)^{m+n-1} \{ (B)^n, (A)^m \}_L
\]

The iterated commutators (eqs. (9) and (10)) consist of a sum of products each having \( m \) factors of \( A \) and \( n \) factors of \( B \); they describe the commutation of a power of one operator with a power of another operator. From equations (6), (7), and (8) follow directly the reduction formulas

\[
\{ (A)^m, (B)^n \} = \sum_{r=1}^{n} \sum_{t=1}^{m} \binom{n}{r} \binom{m-1}{t-1} \{ (A)^{m-t}, (B)^{n-r} \} \{ (A)^t, (B)^r \}_R
\]

\[
\{ (A^n), (B)^m \} = \sum_{r=1}^{n} \sum_{t=1}^{m} \binom{n}{r} \binom{m-1}{t-1} \{ (A)^{r-t}, (B)^t \}_L \{ (A^{n-r}), (B)^{m-t} \}
\]

Equations (7a) and (12), for example, convert any polynomial in \( A \) and \( B \) into a sum of terms, each of which is a product of iterated commutators and an ordered product \( A^m B^n \).

If \( A \) is the differentiation operator with respect to a parameter on which the operator \( B \) depends, then equation (3) becomes the \( n^{th} \) derivative of \( B \), that is,

\[
\frac{d^n B}{dt^n} = \left( \left( \frac{d}{dt} \right)^n, (B) \right)
\]
and equation (9) describes the commutation properties of the derivatives with the powers of \( B \),

\[
\left\{ \left( \frac{d}{dt} \right)^m, (B)^n \right\}_L = \left\{ \left( \frac{d^m B}{dt^m} \right), (B)^{n-1} \right\}
\]

Employing in turn the identities \([A, B]^\dagger = -[A^\dagger, B^\dagger]\) and equation (10) gives the following for the Hermitian adjoint:

\[
\left\{ (A)^m, (B)^n \right\}_L = (-1)^{m+n-1} \left\{ (A^\dagger)^m, (B^\dagger)^n \right\}_L
\]

(15)

\[
\left\{ (A)^m, (B)^n \right\}_L = (B)^n, (A)^m \right\}_R
\]

(16)

**EXPANSION IN ITERATED COMMUATORS**

First some useful disentangling expressions involving the quantities \((A_1 + B_0)^n\) will be developed. These "ordered powers" of \((A + B)\) are simply

\[
(A_1 + B_0)^n = \sum_{r=0}^{n} \binom{n}{r} A^{n-r} B^r
\]

(17)

that is, they are obtained as ordinary binomial expansions in which \(A_1\) and \(B_0\) are treated as though they commuted. When each term is written in the usual positional convention, powers of \(A\) appear always to the left of powers of \(B\). Multiplying both sides of equation (17) from the left by \((A + B)\) gives

\[
(A_2 + B_2)(A_1 + B_0)^n = (A_1 + B_0)^{n+1} - \sum_{r=1}^{n} \binom{n}{r-1}[A^{n+1-r}, B]B^{r-1}
\]

(18)

where, for convenience, both notations have been used on the right. After using, in succession, equations (7b), (6), (7a), and (9), the second term on the right-hand side of equation (18) becomes

\[
\sum_{r=1}^{n} \sum_{t=1}^{n+1-r} \sum_{p=0}^{r-1} (-1)^t \binom{n}{r-1} \binom{t}{r-1} \binom{r-1}{p} A^{n+1-r-t} B^{r-1-p} \left\{ (A)^t, (B)^{p+1} \right\}_L
\]
The substitutions \( j = p + t, \ k = t - 1 \) and \( \ell = n + 1 - r - t \) separate the summation into independent sums over \( \ell \) and \( k \). The result allows equation (18) to be written in the form

\[
(A_2 + B_2)(A_1 + B_0)^n = (A_1 + B_0)^{n+1} - \sum_{j=1}^{n} \binom{n}{j} (A_1 + B_0)^{n-j} G(j)
\]  

(19)

where

\[
G(j) = \sum_{k=0}^{j-1} (-1)^k \binom{j}{k+1} (A)^{k+1} (B)^{j-k}_L
\]  

(20)

The operator \( G(j) \) is a homogeneous polynomial of degree \((j + 1)\) in the operators \(A\) and \(B\). The subscript \( j \) is bracketed to signify that it has no ordering significance. It is found, for example, that

\[
G(1) = [A, B]
\]

\[
G(2) = 2 \{(A), (B)^2\} - \{(A)^2, (B)\}
\]

\[
G(3) = 3 \{(A), (B)^3\} - 3 \{(A)^2, (B)^2\}_L + \{(A)^3, (B)\}
\]

\[
G(4) = 4 \{(A), (B)^4\} - 6 \{(A)^2, (B)^3\}_L + 4 \{(A)^3, (B)^2\}_L - \{(A)^4, (B)\}
\]

On the right-hand side of equation (19), all the iterated commutators (eq. (9)) whose indices \( m \) and \( n \) add up to the same value appear in the single operator (eq. (20)) for which \( j = m + n - 1 \) and in none of the others. If only a finite number of iterated commutators are nonvanishing, then all \( G(j) \) with values of \( j \) larger than a certain value will vanish. As an illustration, consider the case where \( A \) is proportional to \( p^2 \), \( B \) is a polynomial in \( x \) of degree \( \ell \), and \([p, x] = c\), an ordinary number. With the help of the identity

\[
[p^m, x^\ell] = \sum_{r=1}^{m} \binom{m}{r} \ell(\ell - 1) \ldots (\ell - r + 1)c^r x^{\ell-r} p^{m-r}
\]

it is found that
\[ \{ (p^2)^m, (x^l) \} = \sum_{r=0}^{m} q_r(x) p^r \]

where \( q_r(x) \) is a polynomial in \( x \) of degree \( l - 2m + r \). The iterated commutator vanishes if \( m > l \). On the other hand, when \( m \leq l \), \( \{ (p^2)^m, (x^l)^{1-m+1} \} \) vanishes if \( j \geq 2m + 1 \). Hence, when \( j \geq 2l + 1 \), each left commutator (eq. (9)) appearing in \( G(j) \) vanishes and \( G(j) = 0 \).

With the help of the recursion relation (eq. (19)), the following disentangling formula can be verified directly by induction:

\[ (A_1 + B_0)^n - (A + B)^n \]

\[ = \sum_{r=1}^{n-1} \binom{n}{r+1} (A + B)^{n-1-r} G(r) + \sum_{r=2}^{n-2} \sum_{i+j=r} \binom{n}{r+2} \binom{r+1}{j} (A + B)^{n-2-r} G(i) G(j) \]

\[ + \sum_{r=3}^{n-3} \sum_{h+i+j=r} \binom{n}{r+3} \binom{r+2}{j} \binom{h+i+1}{i} (A + B)^{n-3-r} G(h) G(i) G(j) \]

\[ + \sum_{r=4}^{n-4} \sum_{g+h+i+j=r} \binom{n}{r+4} \binom{r+3}{j} \binom{g+h+1}{i} \binom{g+h+i+1}{h} (A + B)^{n-4-r} G(g) G(h) G(i) G(j) \]

\[ + \ldots + S_N \]  \quad (21)

The number \( N \) of summation terms on the right equals the largest integer that is less than or equal to \((1/2)n\). The final term \( S_N \) is \((n - 1)(n - 3) \ldots (5)(3)[G(1)](1/2)n\), when \( n \) is even, and is the sum term for \( r \) equal to \((1/2)(n \pm 1)\), when \( n \) is odd. A dual form of equation (21) holds, with ordered powers of \((A + B)\) appearing on the right in place of ordinary powers:
\[(A_1 + B_0)^n - (A + B)^n\]

\[= \sum_{r=1}^{n-1} \binom{n}{r+1} (A_1 + B_0)^{n-1-r} G_r \sum_{r=2}^{n-2} \sum_{i+j=r} \binom{n}{r+1} (A_1 + B_0)^{n-2-r} G_j G_i \]

\[+ \sum_{r=3}^{n-3} \sum_{h+i+j=r} \binom{n}{r+2} \binom{h+i+1}{j} (A_1 + B_0)^{n-3-r} G_j G_i G_h + \ldots + (-1)^{N-1} S_N \]  \hspace{1cm} (22)

The form of the dual expression (eq. (22)) is similar to equation (21) except that (1) the order of the subscripts on the \( G_j \) factors is reversed and (2) the sign on successive sum terms alternates, beginning with a plus sign on the first term.

The order of the operator factors in each term of equation (21) can be reversed by taking the Hermitian adjoint of each side. The Hermitian adjoint of a functional that is written in the Feynman notation is gotten by replacing every operator \( A(s) \) by \( A^\dagger(s) \) and exactly reversing the ordering convention on the parameters of the adjoint operators.

For a simple function of operators, the result is clearly \( F(A_1, B_0)^\dagger = F(A_0^\dagger, B_1^\dagger) \). Equation (15) shows that \( G_j^\dagger \) is obtained from the form (20) by substituting \( A^\dagger, B^\dagger \) for \( A, B \) respectively, and inserting an overall factor of \((-1)^j \). If \( A \) and \( B \) are Hermitian, then \( G_j^\dagger = (-1)^j G_j \).

The application of equations (21) and (22) to analytic functions of \( (A + B) \) is straightforward. Let the analytic function be

\[F(x) = \sum_{n=0}^{\infty} \frac{1}{n!} f_n x^n \]  \hspace{1cm} (23)

In the formula

\[F[\lambda(A + B)] = F[\lambda(A_1 + B_0)] + R \]  \hspace{1cm} (24)

the term \( R \) has the series expansion

\[R = \left(\frac{\lambda^2}{2!}\right) R_{(1)} + \left(\frac{\lambda^3}{3!}\right) R_{(2)} + \left(\frac{\lambda^4}{4!}\right) R_{(3)} + \ldots \]  \hspace{1cm} (25)
Equation (22) gives the operator \( R(n) \) directly in terms of the constant \( f_n \), ordered powers of \((A + B)\), and the \( G(j)\). An alternative formulation is the disentangling formula

\[
F[\lambda(A_1 + B_0)] = F[\lambda(A + B)]P
\]

where

\[
P = 1 + \left(\frac{\lambda}{2!}\right)P(1) + \left(\frac{\lambda^2}{3!}\right)P(2) + \left(\frac{\lambda^3}{4!}\right)P(3) + \ldots
\]

Equating the coefficients of like powers of \( \lambda \) in equation (26), with the help of equation (21), yields the operators \( P(n) \). The first few terms are

\[
P(1) = \left(\frac{f_2}{f_0}\right)G(1)
\]

\[
P(2) = \left(\frac{f_3}{f_0}\right)G(2) + 3f_0^{-2}(f_0f_3 - f_1f_2)(A + B)G(1)
\]

\[
P(3) = \left(\frac{f_4}{f_0}\right)G(3) + 4f_0^{-2}(f_0f_4 - f_1f_3)(A + B)G(2) + 6f_0^{-3}\left[f_0^2 - f_0^2 - 2f_1(f_0f_3 - f_1f_2)\right](A + B)G(1)
\]

A dual form of equation (26) can also be developed, namely,

\[
F[\lambda(A + B)] = F[\lambda(A_1 + B_0)]P^{-1}
\]

where \( P^{-1} \) is expressed in terms of ordered powers of \((A + B)\). Other expansion methods for analytic functions of \((A + B)\) and references to earlier work in this area are given by Kumar (ref. 3).

## EXPONENTIAL FUNCTIONS

The operators \( P(n) \) in equation (27) take a particularly simple form when \( F \) is the exponential function, in which case \( f_n = 1 \) for all values of \( n \). This leads to a compact statement of the theorem

\[
\exp(\lambda A)\exp(\lambda B) = \exp(\lambda(A + B))\exp(C)
\]
where

\[ C = \left( \frac{\lambda^2}{2!} \right) E(1) + \left( \frac{\lambda^3}{3!} \right) E(2) + \left( \frac{\lambda^4}{4!} \right) E(3) + \cdots \]  
(30)

If equation (29) is written in the form

\[ \exp[\lambda(A_1 + B_0)] - \exp[\lambda(A + B)] = \exp[\lambda(A + B)][\exp(C) - 1] \]  
(31)

the coefficient of \((\lambda^n/n!\)) in the power series expansion of the left-hand side is given by equation (21). The corresponding coefficient on the right is

\[ \sum_{m=1}^{N} \sum_{r=m}^{n-m} \sum_{a+b+\ldots+i+j=r} \frac{1}{m!} \left( \frac{n}{r+m} \right) \left( \frac{r+m}{a+1} \right) \ldots \left( \frac{h+i+j+3}{h+1} \right) \left( \frac{i+j+2}{i+1} \right) \]

\[ \times (A + B)^{n-r-m} E(a) E(b) \ldots E(h) E(i) E(j) \]  
(32)

In the \(m\)th product term of the previous sum (eq. (32)), there appear \(m\) factors of \(E(j)\) and \(m\) binomial coefficients. The \(E(j)\) are found by equating coefficients of the same power of \(\lambda\) on each side of equation (31). The results through ninth order in \(\lambda\) are

\[ E(1) = G(1), \quad i = 1, 2, 3 \]

\[ E(4) = G(4) + \left[ G(1), G(2) \right] \]

\[ E(5) = G(5) + \left( \frac{5}{2} \right) \left[ G(1), G(3) \right] \]

\[ E(6) = G(6) + \left( \frac{9}{2} \right) \left[ G(1), G(4) \right] + \left( \frac{5}{2} \right) \left[ G(2), G(3) \right] - \left( \frac{1}{2} \right) \left[ \left( G(1) \right)^2, G(2) \right] \]

\[ E(7) = G(7) + 7 \left[ G(1), G(5) \right] + 7 \left[ G(2), G(4) \right] + \left( \frac{14}{3} \right) \left[ \left( G(1) \right)^3, \left( G(2) \right)^2 \right] \]

\[ E(8) = G(8) + 10 \left[ G(1), G(6) \right] + 14 \left[ G(2), G(5) \right] + 7 \left[ G(3), G(4) \right] - 12 \left( \left[ G(1) \right]^3, G(2) \right) \]

\[ + 3 \left( \left[ G(1) \right]^2, G(4) \right) + 18 \left[ G(1), G(2) \right] \left[ G(3) \right] + 10 \left[ G(1), G(3), G(2) \right] \]
Note that each of the terms occurring in $E_{(j)}$ is essentially predetermined to within a numerical coefficient. Consider any single term in the sum of terms that makes up the complete expression for a given $E_{(j)}$. If the subscript on every $G_{(i)}$ appearing in the term has its numerical value increased by unity, then the numbers so obtained add up to $(j + 1)$, the degree of the iterated commutators in $G_{(j)}$.

The formula of Zassenhaus (ref. 4)

$$\exp[\lambda(A + B)] = \exp(\lambda A)\exp(\lambda B)\exp\left(\frac{\lambda^2 C_{(2)}}{2!}\right)\exp\left(\frac{\lambda^3 C_{(3)}}{3!}\right)\ldots \quad (33)$$

corresponds to the complete factorization of $\exp(-C)$ in the inverse form of equation (29). With the help of equation (22), the operators $C_{(j)}$ are obtained by equating coefficients of like powers of $\lambda$. Again, the results out to the ninth order in $\lambda$ are

$$C_{(1)} = -G_{(1)}; \quad i = 1, 2, 3$$
$$C_{(4)} = -G_{(4)} - 6[G_{(1)}, G_{(2)}]$$
$$C_{(5)} = -G_{(5)} - 10[G_{(1)}, G_{(3)}]$$
$$C_{(6)} = -G_{(6)} - 15[G_{(1)}, G_{(4)}] - 20[G_{(2)}, G_{(3)}] - 45\left\{G_{(1)}^2, G_{(2)}\right\}$$
$$C_{(7)} = -G_{(7)} - 21[G_{(1)}, G_{(5)}] - 35[G_{(2)}, G_{(4)}] + 210\left\{(G_{(1)}), (G_{(2)})^2\right\} - 105\left\{(G_{(1)})^2, (G_{(3)})\right\}$$
$$C_{(8)} = -G_{(8)} - 28[G_{(1)}, G_{(6)}] - 56[G_{(2)}, G_{(5)}] - 70[G_{(3)}, G_{(4)}] - 210\left\{(G_{(1)}), (G_{(4)})\right\}$$
$$-420\left\{G_{(1)}^3, (G_{(2)})\right\} + 420\left[G_{(1)}, G_{(2)}, G_{(3)}\right] + 560\left[G_{(1)}, G_{(3)}; G_{(2)}\right]$$

Because of the Jacobi and other identities, the expressions given for the operators $E_{(j)}$ and $C_{(j)}$ are not altogether unique. However, they display concisely the iterated-commutator nature of the terms in the expansions of equations (30) and (33). No attempt has been made to obtain general expressions. Nevertheless, for certain types of terms, the general form of the numerical coefficients can be inferred from the specific values already given. For example, $C_{(j)}$ contains the term $(-1/2)(j - 1)[G_{(1)}, G_{(j-2)}]$.

This procedure may also be applied to the Baker-Campbell-Hausdorff (BCH) formula

$$\exp(\lambda A)\exp(\lambda B) = \exp(H), \quad (34)$$

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where
\[ H = \lambda H_0 + \left( \frac{\lambda^2}{2!} \right) H_1 + \left( \frac{\lambda^3}{3!} \right) H_2 + \ldots \]  \hspace{1cm} (35)

\[ H_0 = A + B \]

In the case of the BCH formula, the method offers no great advantage over previous methods (refs. 4 and 5) that have been developed specifically for this problem. However, the \( H(j) \) can be computed within the framework of the procedure given herein without introducing additional elements (such as operator derivatives or auxiliary operator functions) that the more specialized methods employ. Equating the coefficient of \( (\lambda^n/n!) \) in the expansions of \[ \exp(\lambda H) - \exp(\lambda H_0) \] to the expression given by equation (21) yields

\[ H_1 = G(1) \]

\[ H_2 = G(2) + \left( \frac{3}{2} \right) [H_0, G(1)] \]

\[ H_3 = G(3) + 2[H_0, G(2)] + \{(H_0)^2, G(1)\} \]

\[ H_4 = G(4) + \left( \frac{5}{2} \right) [H_0, G(3)] + [G(1), G(2)] + \left( \frac{5}{3} \right) \{(H_0)^2, (G(1))^2\} + \left( \frac{5}{2} \right) \{(H_0), (G(1))^2\} \]

\[ H_5 = G(5) + 3[H_0, G(4)] + \left( \frac{5}{2} \right) [G(1), G(3)] + \left( \frac{5}{3} \right) \{(H_0)^2, (G(3))\} + 8[H_0, G(1), G(2)] \]

\[ + 2[H_0, G(2), G(1)] + \{(H_0)^2, (G(1))^2\} + \left( \frac{1}{2} \right) \{(H_0)^4, (G(1))\} \]

When expressed in terms of the \( G(j) \), the \( H(j) \) contain considerably more terms than either the \( E(j) \) or the \( C(j) \). The additional terms are the ones containing \( H_0 \). Moreover, the relations

\[ G(2) = \{(A, B)^2\} + [G(1), H_0] \]

and

\[ \text{No such simple relations exist for higher } G(j), \text{ however.} \]
\[ G_{(3)} = \{ (A), (B) \}^3 + [G_{(2)}, H_0] \]

can be used to reduce the expressions for the \( H_{(j)} \). For example, the following can be written:

\[ H_{(2)} = \left( \frac{1}{2} \right) \{ (A), (B) \}^2 + \left( \frac{1}{2} \right) (A)^2, (B) \]

\[ H_{(3)} = \{ (A)^2, (B)^2 \}_L \]

There exist any number of intermediate formulas between the BCH form (eq. (34)) and equation (29), all of which can be written as

\[ \exp(\lambda A)\exp(\lambda B) = \exp \left[ \lambda H_0 + \left( \frac{\lambda^2}{2!} \right) H_{(1)} + \ldots + \left( \frac{\lambda^n}{n!} \right) H_{(n-1)} \right] \exp \left[ \frac{\lambda^{n+1}}{(n+1)!} I(n) + \ldots \right] \quad (36) \]

with equation (29) by \( n = 1 \) and equation (33) by the limit \( n \to \infty \). The operators on the right-hand side of equation (35) can be evaluated by the procedure given herein. In particular, the operators in the first exponential on the right are those of the BCH formula, as follows directly from the fact that the right-hand-side expansions of equations (34) and (36) are the same up to the \( n^{th} \) power of \( \lambda \).

Lewis Research Center,
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REFERENCES


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