Letter

Explicit description of the Zassenhaus formula

Tetsuji Kimura$^{1,2,*}$

$^1$Research and Education Center for Natural Sciences, Keio University, Hiyoshi 4-1-1, Yokohama, Kanagawa 223-8521, Japan

$^2$Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan

$^*$E-mail: tetsuji.kimura@keio.jp

Received March 1, 2017; Revised March 19, 2017; Accepted March 21, 2017; Published April 27, 2017

We explicitly describe an expansion of $e^{A+B}$ as an infinite sum of the products of $B$ multiplied by the exponential function of $A$. This is the explicit description of the Zassenhaus formula. We also express the Baker–Campbell–Hausdorff formula in a different manner.

Subject Index A13, B80

1. Introduction In various topics in physics and mathematics, we often have to expand the exponential function of two operators $A$ and $B$ such as $e^{A+B}$ in a certain situation (see, for instance, Refs. [1,2]). Such an expansion is described as the Zassenhaus formula ([3] and references therein):

$$e^{t(A+B)} = e^{tA} e^{tB} \prod_{n=2}^{\infty} e^{t^n Z_{n}(A,B)}, \quad (1a)$$

$$Z_n = \frac{1}{n!} \left\{ \frac{d^n}{dt^n} \left( e^{-t^n Z_{n-1} \cdots e^{-t^2 Z_2 e^{-t A} e^{-t B} e^{-t (A+B)}}} \right) \right\}_{t=0}. \quad (1b)$$

Its transposed version is also given as

$$e^{\beta(A+B)} = \left( \prod_{n=2}^{\infty} e^{\beta^n Z_{n}} \right) e^{\beta B} e^{\beta A}, \quad (2a)$$

$$Z_n = \frac{1}{n!} \left\{ \frac{d^n}{d\beta^n} \left( e^{\beta(A+B)} e^{-\beta A} e^{-\beta B} e^{-\beta^2 Z_2} \cdots e^{-\beta^{n-1} Z_{n-1}} \right) \right\}_{\beta=0}. \quad (2b)$$

Unfortunately, however, the above two expressions are rather complicated because we sequentially obtain the explicit expression of higher-order terms in the operators $A$ and $B$. In this paper, we will obtain a new description of the Zassenhaus formula in which all of the higher-order terms are explicitly expressed.

2. Derivation First of all, we expand $(A + B)^n$ and move all the operator $A$ instances to the right in each term, and define the following expression:

$$(A + B)^n = \sum_{m=0}^{n} \frac{n!}{m!(n-m)!} X_m A^{n-m}, \quad (3)$$
where $X_m$ are polynomials involving $B^j$, commutators $[A, [A, \cdots [A, B]]$, and their multiplications. By using $X_m$, we obtain the exponential function of $A + B$ as the following form:

$$e^{A+B} = \sum_{n=0}^{\infty} \frac{1}{n!} (A + B)^n = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{1}{m!(n-m)!} X_m A^{n-m} = \left( \sum_{m=0}^{\infty} \frac{1}{m!} X_m \right) e^A. \quad (4)$$

There exists a recursion relation among $X_m$ in such a way that

$$X_{m+1} = \mathcal{L}_A X_m + BX_m, \quad X_0 = 1, \quad X_1 = B, \quad (5)$$

where $\mathcal{L}_A O$ is the commutator between $A$ and a certain operator $O$ such as $\mathcal{L}_A O = [A, O]$. It is easy to derive Eq. (5) when we compute $(A + B)^{n+1}$ as the product of $(A + B)$ and $(A + B)^n$ in terms of Eq. (3). Let us evaluate the relation (5). It is convenient to express $X_m$ as the sum of new polynomials $X_{m,p}$:

$$X_m = \sum_{p=1}^{m} X_{m,p}, \quad (6)$$

where $p$ denotes the power of $B$ in $X_{m,p}$; an example can be seen in section 3. Substituting the expression (6) into the relation (5), we find three recursion relations:

$$X_{m+1,1} = \mathcal{L}_A X_{m,1}, \quad (7a)$$

$$X_{m+1,m+1} = BX_{m,m}, \quad (7b)$$

$$X_{m+1,p} = \mathcal{L}_A X_{m,p} + BX_{m,p-1}, \quad m \geq p. \quad (7c)$$

We immediately obtain the solutions of these relations (the proof is given in section 3):

$$X_{m,1} = (\mathcal{L}_A)^{m-1} X_{1,1} = (\mathcal{L}_A)^{m-1} B = \mathcal{B}_m', \quad (8a)$$

$$X_{m,m} = B^{m-1} X_{1,1} = B^m, \quad (8b)$$

$$X_{m,p} = \sum_{k=1}^{m-p+1} \frac{(m-1)!}{(k-1)!(m-k)!} X_{m-k,p-1} \mathcal{B}_k'. \quad (8c)$$

Here we introduced the terminology $\mathcal{B}_m'$ defined above. The solution (8c) can be described in an explicit way if we iteratively use Eq. (8c) until we reach $X_{m-(k_1+\cdots+k_{p-1}),1} = \mathcal{B}_m'(k_1+\cdots+k_{p-1})$ given by Eq. (8a). Hence we obtain

$$X_{m,p} = \sum_{k_1=1}^{m-p+1} \sum_{k_2=1}^{m-k_1-p+2} \cdots \sum_{k_{p-1}=1}^{m-(k_1+\cdots+k_{p-2})-1} \frac{m! \cdot k_1 k_2 \cdots k_{p-1}}{m(m-k_1)(m-k_1-k_2)\cdots(m-(k_1+\cdots+k_{p-2}))} \mathcal{B}_m'(k_1+\cdots+k_{p-1}) \mathcal{B}_{k_2} \cdots \mathcal{B}_{k_1}. \quad (9)$$

For simplicity, we further introduced the description $\mathcal{B}_m \equiv \frac{1}{m!} \mathcal{B}_m'$. Applying Eq. (9) to Eq. (3) and Eq. (6), we obtain the explicit expansion of $e^{A+B}$ in terms of the products of $\mathcal{B}_m'$:

$$e^{A+B} = \left( \sum_{m=0}^{\infty} \frac{1}{m!} X_m \right) e^A = \left( 1 + \sum_{m=1}^{\infty} \sum_{p=1}^{m} \frac{1}{m!} X_{m,p} \right) e^A.$$
We note that each

In the same way, the explicit forms of

we have to obtain the explicit expression of all

consider

obtained from Eq. (11) when we extract the terms of the products only of

\( k_i \)

\( X_m \)

at a certain level such as

\( l = \sum_{l=0}^{m-1} k_l \).

Furthermore, if we transpose Eq. (11) and rename

\( A^T \) and \( B^T \) to \( A \) and \( B \), we obtain

\[
e^{A+B} = e^A \left\{ 1 + \sum_{p=1}^{\infty} \sum_{n_1, \ldots, n_p=1}^{\infty} \frac{(-1)^{(n_p+\cdots+n_l)-p} n_p \cdots n_1}{n_p(n_p+n_{p-1}) \cdots (n_p+\cdots+n_1)} B_{n_1} \cdots B_{n_p} \right\}. \tag{12}
\]

This is the explicit description of Eq. (1) without using the functions \( Z_m \). We should notice that the ordering of the operators \( B_{n_i} \) is different from that of Eq. (11).

The descriptions we have obtained are quite useful if the product of the operator \( B_{n_i} \) is truncated at a certain level such as \( B_{n_2} B_{n_{k-1}} \cdots B_{n_1} = 0 \), which originates from the nilpotency of the operator \( B \) of degree \( k \), i.e., \( B^k = 0 \).

3. \( X_{m,p} \) example

Here we explicitly exhibit a series of \( X_{m,p} \) as defined in Eq. (6). When we consider \((A+B)^2\) as the form (3), we obtain \( X_2 \) and \( X_{2,p} \) as follows:

\[
X_2 = B^2 + B' \quad \text{and} \quad X_{2,1} = B'_2, \quad X_{2,2} = B^2.
\]

In the case of \((A+B)^3\), the components \( X_{3,p} \) are

\[
X_{3,1} = B'_3, \quad X_{3,2} = B'_2 B + 2B'B'_2, \quad X_{3,3} = B^3.
\]

In the same way, the explicit forms of \( X_{4,p} \) and \( X_{5,p} \) are given as

\[
X_{4,1} = B'_4, \quad X_{4,2} = B'_3 B + 3(B'_2)^2 + 3B'B'_3, \\
X_{4,3} = (B'_2 B + 2B'B'_2) B + 3B^2 B' \quad \text{and} \quad X_{4,4} = B^4, \\
X_{5,1} = B'_5.
\]
The final form is nothing but \(Xm\).

\[L(BCH, \text{for short})\] formula

4. **Baker–Campbell–Hausdorff formula** We can also discuss the Baker–Campbell–Hausdorff (BCH, for short) formula

\[
e^Z = e^X e^Y = \exp \left\{ X + Y + \frac{1}{2} [X, Y] + \frac{1}{12} ([X, [X, Y]] + [Y, [Y, X]]) + \cdots \right\}, \quad (13)
\]

by using the descriptions (11) and (12), though the general form (13) is already well known (see, for instance, Ref. [4]). We would like to use the operator \(e^Z\) rather than \(Z\), because we often encounter the exponential form such as \(e^X e^Y\) in quantum mechanics. Multiplying Eq. (11) by \(e^{-A}\) from the right and replacing \(A + B\) and \(−A\) with \(X\) and \(Y\) respectively, we obtain

\[
e^X e^Y = 1 + \sum_{p=1}^{\infty} \sum_{n_p, \ldots, n_1=1}^{\infty} \frac{(-1)^{\sum_{i=1}^{p} n_i}}{n_p (n_p + n_{p-1}) \cdots (n_p + \cdots + 1)} X_{n_p} \cdots X_{n_1}, \quad (14a)
\]

and

\[
X_n = \frac{1}{n!} (L_Y)^{n-1} (X + Y). \quad (14b)
\]
On the other hand, multiplying Eq. (12) by $e^{-A}$ from the left and replacing $-A$ and $A + B$ with $X$ and $Y$ respectively, we find

$$e^X e^Y = 1 + \sum_{p=1}^{\infty} \sum_{n_1, \ldots, n_p=1}^{\infty} \frac{n_p \cdots n_1}{n_p(n_p + n_{p-1}) \cdots (n_p + \cdots + n_1)} y_{n_1} \cdots y_{n_p},$$

or

$$y_n = \frac{1}{n!} (L_X)^{n-1} (X + Y).$$  \hspace{1cm} (15b)

The original BCH formula $Z = \log(e^X e^Y)$ consists only of $X$, $Y$, and their commutators. On the other hand, we immediately find that powers of $X$ and $Y$ directly contribute to the expansion in both Eqs. (14) and (15). These two seem to be different features. However, the powers of $X$ and $Y$ in Eqs. (14) and (15) originate from the corresponding power of $X + Y$ in the Taylor expansion of Eq. (13).

We recognize that the operators $X$ and $Y$ in Eqs. (14) and (15) do not appear on an equal footing with each other. In order to describe an expression on an equal footing, we simply sum Eqs. (14) and (15), and divide it by two. For instance, we evaluate this up to cubic powers of the operators $X$ and $Y$ in such a way that

$$\frac{1}{2} [(14) + (15)] = \frac{1}{2} \left[ 1 + (X_1 - X_2 + X_3 + \cdots) + \left( \frac{1}{2} X_1 X_1 - \frac{1}{3} X_2 X_1 - \frac{2}{3} X_1 X_2 + \cdots \right) \right]$$

$$+ \left( \frac{1}{6} X_1 X_1 + \cdots \right) + \frac{1}{2} \left[ 1 + (Y_1 + Y_2 + Y_3 + \cdots) \right]$$

$$+ \left( \frac{1}{2} Y_1 Y_1 + \frac{2}{3} Y_2 Y_1 + \frac{1}{3} Y_1 Y_2 + \cdots \right) + \left( \frac{1}{6} Y_1 Y_1 + \cdots \right) \right]$$

$$= 1 + (X + Y) - \frac{1}{4} ([Y, X] - [X, Y]) + \frac{1}{12} ([Y, [Y, X]] + [X, [X, Y]])$$

$$+ \frac{1}{2} (X + Y)^2 - \frac{1}{12} ([Y, X] (X + Y) - (X + Y) [X, Y])$$

$$- \frac{1}{6} (X + Y) [Y, X] - [X, Y] (X + Y) + \frac{1}{6} (X + Y)^3 + \cdots$$

$$= 1 + (X + Y) + \left\{ \frac{1}{2} [X, Y] + \frac{1}{2} (X + Y)^2 \right\} + \left\{ \frac{1}{12} ([Y, [Y, X]] + [X, [X, Y]]) \right\}$$

$$+ \frac{1}{4} ([X, Y] (X + Y) + (X + Y) [X, Y]) + \frac{1}{3!} (X + Y)^3 + \cdots$$

This coincides with the Taylor expansion of $e^X e^Y$ in the form of Eq. (13). Indeed, we can find the coincidence in any powers of the operators. Once we establish the above new descriptions, it would be interesting to apply it to a generalization of the BCH formula such as $e^X e^Y e^Z$ developed in Refs. [5–7].

Acknowledgements

I would like to thank Reona Arai, Tetsutaro Higaki, Hideaki Iida, Hiroyasu Miyazaki, Toshifumi Noumi, Noriaki Ogawa, Masato Taki, Akinori Tanaka, and Masahide Yamaguchi for helpful discussions. I would also like to thank Katsushi Ito, Marco Matone, and Hector Moya-Cessa for valuable correspondence. I am supported by the Iwanami-Fujukai Foundation. I am also supported in part by the MEXT-Supported Program for the Strategic Research Foundation at Private Universities “Topological Science” (Grant No. S1511006)
and by the MEXT Grant-in-Aid for Scientific Research on Innovative Areas “Nuclear Matter in Neutron Stars Investigated by Experiments and Astronomical Observations” (No. 15H00841 by Muneto Nitta).

References

[1] J. Martínez-Carranza, F. Soto-Eguibar, and H. Moya-Cessa, Eur. Phys. J. D 66, 22 (2012).
[2] T. Kimura, A. Mazumdar, T. Noumi, and M. Yamaguchi, J. High Energy Phys. 1610, 022 (2016) [arXiv:1608.01652 [hep-th]] [Search INSPiRE].
[3] F. Casas, A. Murua, and M. Nadinic, Comput. Phys. Commun. 183, 2386 (2012) [arXiv:1204.0389 [math-ph]] [Search INSPiRE].
[4] V. S. Varadarajan, Lie Groups, Lie Algebras, and their Representations (Springer-Verlag, New York, 1984).
[5] M. Matone, J. High Energy Phys. 1505, 113 (2015) [arXiv:1502.06589 [math-ph]] [Search INSPiRE].
[6] M. Matone, J. Geom. Phys. 97, 34 (2015) [arXiv:1503.08198 [math-ph]] [Search INSPiRE].
[7] M. Matone, Eur. Phys. J. C 76, 610 (2016) [arXiv:1504.05174 [math-ph]] [Search INSPiRE].