Baker-Campbell-Hausdorff Formula

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1 Motivation

The Baker–Campbell–Hausdorff (BCH) formula is worth studying because it's the precise tool that tells you what happens when you compose actions generated by non-commuting operators, a question that is relevant to many problems in physics and engineering. In quantum mechanics it turns products of time-evolution or displacement operators into a single effective generator, with commutator terms that quantify interference and higher-order corrections; in numerical simulation it explains the accuracy of operator-splitting schemes (i.e. Lie–Trotter factorization) by exposing the leading error terms; and in signal processing and electromagnetics it clarifies when exponentials of matrices can be merged without penalty. Here is the famous BCH formula

$$e^A \cdot e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}([A,[A,B]]+[B,[B,A]])+\cdots}$$

where

$$[A,B] \equiv AB - BA$$

We immediately note, that if the commutator, $[A,B] = 0$, the complicated nested commutator terms in the BCH drop out and we obtain

$$a^A e^B = e^{A+B}$$

the expression we are used to from algebra. is the standard commutator between the two operators. In this primer we will proof the BCH formula.

2 Commutators Revisited

We just saw that the complexity of evaluating BCH relies critically on the value of the commutator

$$[A,B] \equiv AB - BA$$

and it is prudent to discuss a few of its properties

$$[A+C,B] = [A,B] + [C,B]$$

which follows directly by resolving the commutator and rearranging

$$\begin{aligned} &[A+C,B] \\ &= (A+C)\,B - B\,(A+C) \\ &= AB + CB - BA - BC \\ &= AB - BA + CB - BC \\ &[A,B] + [C,B] \end{aligned}$$

similarly, we can show that the same linearity holds for the 2nd argument

$$[A,B+C] = [A,B] + [A,C]$$

and if we reverse the arguments

$$[A,B] = -[B,A]$$

3 Nested Commutators and Useful Relationships

In this section we provide the groundwork for the proof of BCH.

3.1 ad_X, a Useful Auxiliary Function

Let's define a useful auxiliary function to describe nested commutators

$$ad_X\,(Y) \equiv [X,Y]$$

let's pause for a moment and explore this notation further. Specifically lets look at powers of the auxiliary function

$$\begin{aligned} &ad_X\,(Y)^2 \\ &= ad_X \circ ad_X\,(Y) \\ &= ad_X\,(ad_X\,(Y)) \\ &= [X,[X,Y]] \end{aligned}$$

in other words, powers of the auxiliary function are resolved via the chain rule, ***not*** as regular products. This difference matters as we can easily confirm by example. Alternatively, we realize that each term in the naive product has the same number of X and Y operators, while the (correct) chain rule resolution only contains a single factor Y. Here is a general term:

$$ad_X^n\,(Y) = \underbrace{[X,[X,\cdots[X,Y]\cdots]]}_{n\;times}$$

note also that the auxiliary function is linear, and we have for example

$$\begin{aligned} A &= \sum A_n \\ ad_A(Z) &= [\sum A_n, Z] \\ &= \sum [A_n, Z] \\ &= \sum ad_{A_n}(Z) \end{aligned}$$

3.2 ad_X for Decomposing Operator Products

Let's decompose the following operator product:

$$f\,(s) \equiv e^{sX} Y e^{-sX}$$

We assume that the operator exponentials are differentiable and we use a Taylor polynomial (see primer on Taylor polynomials and series) to describe the function $f(s)$

$$f(s) = \sum_{n=0}^{\infty} \frac{s^n}{n!} \frac{d^n}{ds^n} f\,(0)$$

let's compute the derivative of $f(s)$

$$\begin{aligned} \frac{d}{ds} f(s) &= f'(s) \\ = X e^{sX} Y e^{-sX} &- e^{sX} Y e^{-sX} X \\ &= X f(s) - f(s) X \\ &= [X, f(s)] \\ &= ad_x(f(s)) \end{aligned}$$

and for the next derivative

$$\begin{aligned} \frac{d^2}{ds^2} f(s) &= f''(s) \\ = X f'(s) &- f'(s) X \\ &= [X, f'(s)] \\ &= ad_x(ads(f(s)) \\ &= ad_x \circ ad_x(f(s)) \\ &= ad_X^2(f(s)) \end{aligned}$$

and repeatedly applying this calculation, we find

$$\frac{d^n}{ds^n} f(s) = ad_X^n(f(s))$$

which evaluates to

$$\frac{d^n}{ds^n}f(0) = ad_X^n(f(0)) = ad_X^n(Y)$$

and putting the terms back into the Taylor expansion, we obtain

$$\begin{aligned} f(s) &= \sum_{n=0}^{\infty} \frac{s^n}{n!} \frac{d^n}{ds^n} f(0) \\ &= \sum_{n=0}^{\infty} \frac{s^n}{n!} ad_X^n(Y) \end{aligned}$$

4 Hadamard Lemma

With these preliminaries we can proof the Hadamard lemma, which states

$$e^X Y e^{-X} = e^{ad_X} \circ Y = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \cdots$$

where $[X, Y] = XY - YX$ is the usual commutator. Note, that the middle expression is evaluated using the chain rule (see section 3). We realize that all we have to do is to evaluate $f(s = 1)$ and unpack the auxiliary function ad_Xfollowing the rules outlined in section 3.1

$$\begin{aligned} f(s = 1) &= e^X Y e^{-X} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} ad_X^n(Y) \\ &= Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \cdots \\ &= e^{ad_X} \circ Y \end{aligned}$$

4.1 Corollary to the Hadamard Lemma

In preparation for the BCH proof we provide here an application of the Hadamard lemma to express the left hand side of BCH

$$U(t) \equiv e^{tA} e^{tB}$$

in terms of powers of the auxiliary, ad_X operator function

$$\begin{aligned}
\dot{U}(t) &= \frac{d}{dt}U(t) \\
&= Ae^{tA}e^{tB} + e^{tA}Be^{tB} \\
&= AU(t) + e^{tA}B\left(e^{-tA}e^{tA}\right)e^{tB} \\
&= AU(t) + e^{tA}Be^{-tA}U(t) \\
\Rightarrow \dot{U}(t)U(t)^{-1} &= A + e^{tA}Be^{-tA} \\
&= A + \sum_{n=0}^{\infty}\frac{t^n}{n!}ad_A^n(B)
\end{aligned}$$

5 Proof of Wilcox/Duhamel Identity

In this section we will proof the Wilcox/Duhamel identity we will use to proof BCH

$$\frac{d}{dt}e^{Z(t)} = \int_0^1 e^{(1-s)Z(t)}\dot{Z}(t)e^{sZ(t)}ds$$

However, in foresight you see that the target (operator) function Z(t) appear on the left and on the right hand side. Thus, we will find our final function through recursion. Let's get started by defining

$$F(s) = e^{(1-s)Y}e^{sX}$$

Now, we compute the derivative

$$\begin{aligned}
\frac{d}{ds}F(s) &= -Ye^{(1-s)Y}e^{sX} + e^{(1-s)Y}Xe^{sX} \\
&= e^{(1-s)Y}\left(X - Y\right)e^{sX}
\end{aligned}$$

and integrate

$$\begin{aligned}
\int_0^1 e^{(1-s)Y}\left(X - Y\right)e^{sX}ds & \\
&= \int_0^1 \frac{d}{ds}F(s)ds \\
&= F(1) - F(0) \\
& e^X - e^Y
\end{aligned}$$

now we specify $X = Z(t+h)$ and $Y = Z(t)$

$$e^{Z(t+h)} - e^{Z(t)} = \int_0^1 e^{(1-s)Z(t)}\left(Z(t+h) - Z(t)\right)e^{sZ(t+h)}ds$$

and we divide both sides by the increment, h, and take the limit $h->0$

$$\lim_{h->0}\frac{e^{Z(t+h)}-e^{Z(t)}}{h} = \lim_{h->0}\int_0^1 e^{(1-s)Z(t)}\frac{(Z(t+h)-Z(t))}{h}e^{sZ(t+h)}ds$$

$$\frac{d}{dt}e^{Z(t)} = \int_0^1 e^{(1-s)Z(t)}\dot{Z}(t)e^{sZ(t)}ds$$

and a corollary we will be using soon, right multiply with e^{-Z} and simplify using the Hadamard lemma

$$\begin{aligned}\left(\frac{d}{dt}e^{Z(t)}\right)e^{-Z(t)} &= \int_0^1 e^{(1-s)Z(t)}\dot{Z}(t)e^{sZ(t)}ds\ e^{-Z(t)}\\ &= \int_0^1 e^{(1-s)Z(t)}\dot{Z}(t)e^{sZ(t)}e^{-Z(t)}ds\\ &= \int_0^1 e^{(1-s)Z(t)}\dot{Z}(t)e^{-(1-s)Z(t)}ds\\ &= \int_0^1 e^{(1-s)ad_Z}\dot{Z}(t)ds\\ &= \sum_{k=0}^{\infty}\frac{1}{(k+1)!}ad_Z^k\left(\dot{Z}\right)\end{aligned}$$

where in the last two steps we used the Hadamard lemma from section 4 and performed the trivial integrals over s.

6 Proof of BCH Formula

At long last we are in a position to proof the BCH formula. We define two new functions, that mimic the structure of the BCH formula, determine a single exponent operator function, $Z(t)$, from from two exponential operator functions, A and B

$$\begin{aligned}U(t) &\equiv e^{Z(t)}\\ &\equiv e^{tA}e^{tB} \Rightarrow Z(0)=0\end{aligned}$$

and put the first definition in the Wilcox/Duhamel identity from section 5

$$\begin{aligned}\dot{U}U^{-1} &= \int_0^1 e^{(1-s)ad_Z}\dot{Z}(t)ds\\ &= \sum_{k=0}^{\infty}\frac{1}{(k+1)!}ad_Z^k\left(\dot{Z}\right)\end{aligned}$$

where in the second line we have inserted a "1" in a suitable operator notation. Now we right-multiply with $U^{-1}(t)$ and use the product decomposition from section 3.2 Now, we take the second definition of $U(t)$

$$U(t) \equiv e^{tA}e^{tB}$$

which owing to the corollary to the Hadamard lemma can be expressed as

$$\dot{U}U^{-1} = A + \sum_{n=0}^{\infty} \frac{t^n}{n!} ad_A^n(B)$$

in essence, we have derived two conditions for $\dot{U}U^{-1}$, one dependent on A and B, and the other dependent on our target function $Z(t)$. Moreover, we realize that the second equation is polynomial in t. Thus, our strategy is going to be to write $Z(t)$ as a polynomial in t (note that the polynomial starts with a linear term), compute analytically the derivative $\dot{Z}$, put the expressions in our two equations, and extract the "coefficients" of $Z(t)$ by comparing equal powers of t on both sides.

$$Z(t) = \sum_{n=1}^{\infty} Z_n t^n$$

$$\dot{Z}(t) = \sum_{n=1}^{\infty} n \cdot Z_n t^{n-1}$$

$$\sum_{k=0}^{\infty} \frac{1}{(k+1)!} ad_Z^k \left(\dot{Z}\right) = A + \sum_{n=0}^{\infty} \frac{t^n}{n!} ad_A^n(B)$$

From this expression we extract power-by-power the coefficient operator function Z_n.

Order t^0(n=0)

Right hand side: $A + B$.
Left hand side:
k =0 terms: $ad_Z^0(\dot{Z}) = \dot{Z}$, and we identify Z_1as the only contributing term.
$k \geqslant 1$ terms: the lowest possible order is 1, and higher orders do not contribute any terms.
Combining terms, we obtain: $Z_1 = A + B$.

Order t^1(n=1)

Right hand side: $[A, B]$.
Left hand side:
$k = 0$ terms: $ad_Z^0 \left(\dot{Z}\right) = \dot{Z} \Rightarrow 2Z_2$.
$k = 1$ terms: $ad_Z^1 \left(\dot{Z}\right) = [Z, \dot{Z}]$,with only possible combination $[Z_1, Z_1] = 0$.
$k \geqslant 2$ terms: the lowest possible order is 2, and higher order terms do not contribute any terms.
Combining terms, we obtain: $Z_2 = \frac{1}{2}[A, B]$.

Order t^2(n=2)

Right hand side: $\frac{1}{2}[A,[A,B]]$.
Left hand side:
$k=0$ terms: $ad_Z^0\left(\dot{Z}\right)=\dot{Z}\Rightarrow 3Z_3$

$k=1$ terms: $\frac{1}{2}ad_Z^1\left(\dot{Z}\right)=\frac{1}{2}[Z,\dot{Z}]=\frac{1}{2}[Z_1t+Z_2t^2+\cdots,Z_1+2Z_2t+3Z_3t^2+\cdots]\Rightarrow\frac{1}{2}\left([Z_1,2Z_2]+[Z_2,Z_1]\right)$

$k\geqslant 2$ terms: the lowest possible order 2 contains the commutator $[Z_1,Z_1]=0$, all other terms are of higher order and do not contribute.

Combining terms, we obtain: $\frac{1}{2}[A,[A,B]]=3Z_3+\frac{1}{2}[Z_1,Z_2]=3Z_3+\frac{1}{2}[A+B,\frac{1}{2}[A,B]]=3Z_3+\frac{1}{4}[A,[A,B]]+\frac{1}{4}[B,[A,B]]$ and we solve for Z_3 and simplify $3Z_3=\frac{1}{2}[A,[A,B]]-\frac{1}{4}[A,[A,B]]-\frac{1}{4}[B,[A,B]]=\frac{1}{4}[A,[A,B]]-\frac{1}{4}[B,[A,B]]=\frac{1}{4}[A,[A,B]]+\frac{1}{4}[B,[B,A]]$, and finally: $Z_3=\frac{1}{12}[A,[A,B]]+\frac{1}{12}[B,[B,A]]$

Higher Orders

The bookkeeping gets more involved with each order, so we stop here and leave it to the inclined reader to explore higher orders on their own or to consult the extensive literature on approaches to find the coefficient operator function Z_n for all powers.

Combining Low Order Terms

Up to cubic nested commuter order we have derived the following formula for the product of exponential operators

$$e^A\cdot e^B=e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}([A,[A,B]]+[B,[B,A]])+\cdots}$$
$$[A,B]=AB-BA$$

in agreement with the formula states the the beginning of this primer. This primer showed you a pathway from commutators to Hadamard, to Wilcox/Duhamel, and finally to BCH via coefficient matching—exactly the tools you will reuse in quantum dynamics, and operator-splitting analysis.

7 Exercises

- Show: $[B,[A,B]]=-[B,[B,A]]$.
- Derive the $n=3$ term in the BCH formula.