The Baker - Campbell - Hausdorff formulas

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The name "Baker-Campbell-Hausdorff" is usually associated with a series of formulas devised to help us manipulate the exponential of operators.

The exponential function e^x is peculiar in that it is the only function satisfying the exponential property

$$e^{x+y} = e^x e^y \tag{1}$$

(other bases can always be converted to this basis. For instance, $2^x = e^{\log 2^x} = e^{x \log 2}$).

In quantum mechanics and other fields we commonly encounter functions of operators which are defined by means of a power series. For instance, if

$$f(x) = \sum_{n=0}^{\infty} c_n x^n \tag{2}$$

for some coefficients c_n, then we may eventually stumble upon $f(\hat{A})$, where $\hat{A}$ is an operator. The quantity $f(\hat{A})$ is always defined by means of a power series

$$f(\hat{A}) = \sum_{n=0}^{\infty} c_n \hat{A}^n \tag{3}$$

The reason is that $\hat{A}^2, \hat{A}^3, \ldots$ are always well defined quantities.

By far the most important example is the exponential, whose
ylor expansion is

$$\boxed{e^{x} = \sum_{m=0}^{\infty} \frac{x^m}{m!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \dots} \qquad (4)$$

The exponential of $\hat{A}$, also called the <u>matrix exponential</u>, is defined analogously

$$\boxed{e^{\hat{A}} = \sum_{m=0}^{\infty} \frac{1}{m!} \hat{A}^m = 1 + \hat{A} + \frac{\hat{A}^2}{2} + \frac{\hat{A}^3}{3!} + \dots} \qquad (5)$$

But now comes a remarkable fact: $e^{\hat{A}}$ does <u>not</u> satisfy the exponential property (1).

$$e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}} \quad \text{(in general)} \qquad (6)$$

A simple way of seeing why is to note that $e^{\hat{A}+\hat{B}} = e^{\hat{B}+\hat{A}}$ so if (6) were true it would imply $e^{\hat{A}} e^{\hat{B}} = e^{\hat{B}} e^{\hat{A}}$; ie, the two operators would commute, which is not necessarily true. In fact, this gives us a hint as to when will $e^{\hat{A}+\hat{B}}$ be equal to $e^{\hat{A}} e^{\hat{B}}$:

$$\boxed{e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} \quad \text{if } [\hat{A}, \hat{B}] = 0} \qquad (7)$$

We shall prove this rigorously in due course. But for now, think a little about whether or not this makes sense.

Before we continue, the following theorem may be useful:

$$\boxed{[\hat{A},\hat{B}]=0 \Rightarrow [\hat{A}, f(\hat{B})]=0 \quad \text{for any } f(x)} \qquad (8)$$

You can prove this using (2).

Our goal is to learn what to do with (6). But first let us develop another formula, which also goes by the name BCH, and is also extremely useful: we want to work out

$$e^{t\hat{A}}\,\hat{B}\,e^{-t\hat{A}}$$

where t is some parameter. If you want you can make $t=1$, or t imaginary or anything you want. But it is useful to keep it there, as you will see.

Now, expanding the exponentials in a series we get

$$e^{t\hat{A}}\hat{B}e^{-t\hat{A}} = \left(1+t\hat{A}+\frac{t^2\hat{A}^2}{2!}+\frac{t^3\hat{A}^3}{3!}+\dots\right)\hat{B}\left(1-t\hat{A}+\frac{t^2\hat{A}^2}{2!}-\frac{t^3\hat{A}^3}{3!}+\dots\right)$$

Now the t will come in handy: when we expand the product we may collect terms of the same order in t:

$$e^{t\hat{A}}\hat{B}e^{-t\hat{A}} = \hat{B} + t(\hat{A}\hat{B}-\hat{B}\hat{A}) + \frac{t^2}{2!}(\hat{A}^2B + \hat{B}\hat{A}^2 - 2\hat{A}\hat{B}\hat{A})$$

$$+\frac{t^3}{3!}(\hat{A}^3\hat{B} - \hat{B}\hat{A}^3 + 3\hat{A}B\hat{A}^2 - 3\hat{A}^2\hat{B}\hat{A}) + \dots$$

We now identify several commutators:

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$[\hat{A},[\hat{A},\hat{B}]] = \hat{A}(\hat{A}\hat{B}-\hat{B}\hat{A}) - (\hat{A}\hat{B}-\hat{B}\hat{A})\hat{A}$$

$$= \hat{A}^2 B - 2\hat{A}\hat{B}\hat{A} + B\hat{A}^2$$

$$[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] = \hat{A}(\hat{A}^2\hat{B} - 2\hat{A}\hat{B}\hat{A} + B\hat{A}^2) - (\hat{A}^2\hat{B} - 2\hat{A}\hat{B}\hat{A} + \hat{B}\hat{A}^2)\hat{A}$$

$$= \hat{A}^3\hat{B} - 2\hat{A}^2\hat{B}\hat{A} + \hat{A}\hat{B}\hat{A}^2 - \hat{A}^2\hat{B}A + 2\hat{A}\hat{B}\hat{A}^2 - \hat{B}\hat{A}^3$$

$$= \hat{A}^3\hat{B} + 3A\hat{B}\hat{A}^2 - 3\hat{A}^2\hat{B}A - \hat{B}\hat{A}^3$$

$$= \hat{A}^3\hat{B}$$

Thus we conclude that

$$\boxed{e^{t\hat{A}}\hat{B}e^{-t\hat{A}} = \hat{B} + t[\hat{A},\hat{B}] + \frac{t^2}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{t^3}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + \ldots} \quad (9)$$

This formula is <u>extremely</u> useful.

If you want a more sucint notation define $\hat{A}^m\{\hat{B}\}$ as the m-th commutator; ie $\hat{A}^0\{\hat{B}\} = \hat{B}$, $\hat{A}^1\{\hat{B}\} = [\hat{A},\hat{B}]$, $\hat{A}^2\{B\} = [\hat{A},[\hat{A},\hat{B}]]$ and so on. Then

$$\boxed{e^{t\hat{A}}\hat{B}e^{-t\hat{A}} = \sum_{m=0}^{\infty} \frac{t^m}{m!}\hat{A}^m\{\hat{B}\}} \quad (10)$$

The series in Eq. (9) truncates if one of the commutators is zero. The most important example is $\hat{x}$ and $\hat{p}$ or $\hat{a}$ and $\hat{a}^{+}$, whose commutator is a constant (or an operator which commutes with both $\hat{A}$ and $\hat{B}$). Thus, suppose

$$[\hat{A}, \hat{B}] = \varkappa, \quad \text{a constant.}$$

Then

$$\boxed{e^{t\hat{A}} \hat{B} e^{-t\hat{A}} = \hat{B} + \varkappa t} \tag{11}$$

<u>Examples</u>: $[\hat{x}, \hat{p}] = i\hbar$. Let us look at

$$e^{i\hat{p}L/\hbar} \hat{x} e^{-i\hat{p}L/\hbar}$$

Here $t = \frac{iL}{\hbar}$, $[\hat{A}, \hat{B}] = [\hat{p}, \hat{x}] = -i\hbar$ so

$$e^{i\hat{p}L/\hbar} \hat{x} e^{-i\hat{p}L/\hbar} = \hat{x} + \frac{iL}{\hbar}(-i\hbar)$$

$$\boxed{e^{i\hat{p}L/\hbar} \hat{x} e^{-i\hat{p}L/\hbar} = \hat{x} + L} \tag{12}$$

Similarly, if we look at $e^{-ik\hat{x}} \hat{p} e^{ik\hat{x}}$ then $t = -ik$ and $[\hat{A}, \hat{B}] = [\hat{x}, \hat{p}] = i\hbar$ so

$$\boxed{e^{-ik\hat{x}} \hat{p} e^{ik\hat{x}} = \hat{p} + \hbar k} \tag{13}$$

xample: $[\hat{a}, \hat{a}^\dagger] = 1$ so

$$e^{t\hat{a}^\dagger}\hat{a}\,e^{-t\hat{a}^\dagger} = \hat{a} + t[\hat{a}^\dagger, \hat{a}] = \hat{a} - t$$

But $[\hat{N}, \hat{a}] = -\hat{a}$ where $\hat{N} = \hat{a}^\dagger\hat{a}$ (show this!)

thus the formula will not truncate

$$e^{t\hat{N}}\hat{a}\,e^{-t\hat{N}} = \hat{a} + t[\hat{N}, \hat{a}] + \frac{t^2}{2}[\hat{N}, [\hat{N}, \hat{a}]] + \frac{t^3}{3!}[\hat{N}, [\hat{N}, [\hat{N}, \hat{a}]]] + \dots$$

$$= \hat{a} - t\hat{a} + \frac{t^2}{2}[\hat{N}, (-\hat{a})] + \frac{t^3}{3!}[\hat{N}, [\hat{N}, (-\hat{a})]] + \dots$$

$$= \hat{a} - t\hat{a} + \frac{t^2}{2}\hat{a} - \frac{t^3}{3!}\hat{a} + \dots$$

$$= \hat{a}\left[1 - t + \frac{t^2}{2} - \frac{t^3}{3!} + \dots\right] =$$

$$= a\,e^{-t}$$

Hence

$$\boxed{e^{t\hat{N}}\hat{a}\,e^{-t\hat{N}} = \hat{a}\,e^{-t}} \qquad (14)$$

This formula is usually written as

$$e^{t\hat{N}}\hat{a} = \hat{a}\,e^{t\hat{N}}\,e^{-t}$$

(I multiplied by e^{tN} on the right). Thus we see that if we want to exchange $e^{t\hat{N}}$ and $\hat{a}$ we get an extra term e^{-t}.

The other BCH formula

We now go back to Eq. (6) and try to figure out how to separate $e^{\hat{A}+\hat{B}}$. It turns out that this problem is harder than it looks. So let us first work out the case where $[\hat{A},\hat{B}]=\gamma$. Then we discuss the general case.

Let us then work out the following product, using (9):

$$e^{t\hat{A}} e^{\hat{B}} e^{-t\hat{A}} = e^{\hat{B}} + t[\hat{A}, e^{\hat{B}}] + \frac{t^2}{2}[\hat{A},[\hat{A}, e^{\hat{B}}]] + \dots$$

But, since $[\hat{A},\hat{B}]=\gamma$, we have

$$[\hat{A},\hat{B}^2] = [\hat{A},\hat{B}]\hat{B} + \hat{B}[\hat{A},\hat{B}] = 2\gamma B$$

$$[\hat{A},\hat{B}^3] = 3\gamma \hat{B}^2$$

$$\vdots$$

$$[\hat{A},\hat{B}^n] = n\gamma \hat{B}^{n-1}$$

This is a derivative:

$$\boxed{[\hat{A},\hat{B}]=\gamma \Rightarrow [\hat{A}, f(\hat{B})] = \gamma f'(\hat{B})} \tag{15}$$

Hence

$$[\hat{A}, e^{\hat{B}}] = \gamma e^{\hat{B}}$$

hen

$$[\hat{A}, [\hat{A}, e^{\hat{B}}]] = [\hat{A}, \gamma e^{\hat{B}}] = \gamma^2 e^{\hat{B}}$$

and so on. Thus we conclude that

$$e^{t\hat{A}} e^{\hat{B}} e^{-t\hat{A}} = e^{\hat{B}} + \gamma t \, e^{\hat{B}} + \frac{\gamma^2 t^2}{2!} e^{\hat{B}} + \dots$$

$$= e^{\hat{B}} e^{\gamma t}$$

$$\therefore \quad \boxed{\begin{array}{c} e^{t\hat{A}} e^{\hat{B}} e^{-t\hat{A}} = e^{\hat{B}} e^{\gamma t} \\ \text{if } [\hat{A}, \hat{B}] = \gamma \end{array}} \qquad (16)$$

We may now manipulate this formula to write

$$e^{t\hat{A}} e^{\hat{B}} = e^{\hat{B}} e^{t\hat{A}} e^{\gamma t}$$

Setting $\gamma = [\hat{A}, \hat{B}]$ and $t = 1$ we finally obtain

$$\boxed{\begin{array}{c} e^{\hat{A}} e^{\hat{B}} = e^{\hat{B}} e^{\hat{A}} e^{[\hat{A}, \hat{B}]} \\ [\hat{A}, \hat{B}] \text{ commute w/ } \hat{A} \text{ and } \hat{B} \end{array}}$$

This is wonderful. Now we know how to change the order.

<u>Example</u>: $[\hat{a}, \hat{a}^{+}] = 1$

$$e^{\lambda \hat{a}} e^{\alpha \hat{a}^{+}} = e^{\alpha \hat{a}^{+}} e^{\lambda \hat{a}} e^{\alpha \lambda}$$

Finally we look at how to separate $e^{\hat{A}+\hat{B}}$ in the case where $[\hat{A},\hat{B}]$ commutes with both $\hat{A}$ and $\hat{B}$. The trick here is as follows. Define

$$f(t) = e^{t(\hat{A}+\hat{B})}$$
$$g(t) = e^{t\hat{A}} e^{t\hat{B}} e^{-t^2 \gamma/2}$$

where $[\hat{A},\hat{B}] = \gamma$. Now I will show that both f and g satisfy the same differential equation with the same initial condition $f(0) = g(0) = 1$. Thus they must be the same. On the one hand

$$f'(t) = (\hat{A}+\hat{B})\, e^{t(\hat{A}+\hat{B})} = (\hat{A}+\hat{B})\, f(t) = f(t)(\hat{A}+\hat{B})$$

on the other

$$g'(t) = \hat{A}\, e^{t\hat{A}} e^{t\hat{B}} e^{-\gamma t^2/2} + e^{t\hat{A}}\, \hat{B}\, e^{t\hat{B}} e^{-\gamma t^2/2} + e^{t\hat{A}} e^{t\hat{B}} (-\gamma t) e^{-\gamma t^2/2}$$

But, because of (9)

$$\hat{A}\, e^{t\hat{B}} = e^{t\hat{B}}\left(\hat{A} - t[\hat{B},\hat{A}]\right) = e^{t\hat{B}}(\hat{A} + \gamma t)$$

Thus

$$g'(t) = e^{t\hat{A}} e^{t\hat{B}} e^{-\gamma t^2/2}(\hat{A} + \gamma t + \hat{B} - \gamma t)$$
$$= g(t)(\hat{A}+\hat{B})$$

Thus, both f and g obey the same Eq., with the same initial conditions. Hence they must be equal

$$\boxed{\begin{gathered} e^{t(\hat{A}+\hat{B})} = e^{t\hat{A}} e^{t\hat{B}} e^{-\frac{t^2}{2}[\hat{A},\hat{B}]} \\ \text{when } [\hat{A},\hat{B}] \text{ commute with } \hat{A} \text{ and } \hat{B} \end{gathered}}$$

This is how we separate the exponential of the sum. The general case, when $[\hat{A},\hat{B}]$ does not commute with $\hat{A}$ and $\hat{B}$, is much more complicated. Just to give you an idea, the result will look like

$$e^{t(\hat{A}+\hat{B})} = e^{t\hat{A}} e^{t\hat{B}} e^{-\frac{t^2}{2}[\hat{A},\hat{B}]} e^{\frac{t^3}{3!}\Gamma_3} e^{-\frac{t^4}{4!}\Gamma_4} \cdots$$

where

$$\Gamma_3 = 2[\hat{B},[\hat{A},\hat{B}]] + [\hat{A},[\hat{A},\hat{B}]]$$

$$\Gamma_4 = [[[\hat{A},\hat{B}],\hat{A}],\hat{A}] + 3[[[A,\hat{B}],\hat{A}],\hat{B}] + 3[[[\hat{A},\hat{B}],\hat{B}],\hat{B}]$$

So you see, things get <u>very</u> complicated.

Example : an important example is to separate $e^{\alpha\hat{a}^{+}+\beta\hat{a}}$ where $[\hat{a},\hat{a}^{+}]=1$. We have

$$e^{\alpha\hat{a}^{+}+\beta\hat{a}} = e^{\alpha\hat{a}^{+}} e^{\beta\hat{a}} e^{-\alpha\beta/2} = e^{\beta\hat{a}} e^{\alpha\hat{a}^{+}} e^{\alpha\beta/2}$$

For instance we may write $\hat{p} = \frac{i p_0}{\sqrt{2}}(\hat{a}^{+}-\hat{a})$ so that

$$\hat{T}_L = e^{i\hat{p}L/\hbar} = \exp\left\{-\frac{p_0 L}{\hbar\sqrt{2}}(\hat{a}^{+}-\hat{a})\right\} = e^{-\alpha(\hat{a}^{+}-\hat{a})}$$

$$= e^{-\alpha\hat{a}^{+}} e^{+\alpha\hat{a}} e^{\alpha^2/2} = e^{+\alpha\hat{a}} e^{-\alpha\hat{a}^{+}} e^{-\alpha^2/2}$$

This is interesting, for instance, if we want to compute $\hat{T}_L|0\rangle$ where $|0\rangle$ is the ground state of the harmonic oscillator. In this case

$$\hat{T}_L|0\rangle = e^{+\alpha^2/2} e^{-\alpha\hat{a}^{+}} e^{+\alpha\hat{a}}|0\rangle$$

But

$$e^{+\alpha\hat{a}}|0\rangle = \left(1+\alpha\hat{a}+\frac{\alpha^2\hat{a}^2}{2!}+\dots\right)|0\rangle$$
$$= |0\rangle$$

as $\hat{a}|0\rangle = 0$. Thus

$$\hat{T}_L|0\rangle = e^{\alpha^2/2} e^{-\alpha\hat{a}^{+}}|0\rangle$$

this is a coherent state : recall that

$$|\alpha\rangle = c\, e^{\alpha\hat{a}^{+}}|0\rangle$$

for a suitable normalization constant.