0.1 Baker-Campbell-Hausdorff の公式 1

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right] + \frac{1}{2!}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] + \cdots \tag{0.1.1}$$

なる式を示す.

Proof. 函数 $f(t)$ を,

$$f(t) \coloneqq \mathrm{e}^{t\hat{A}}\hat{B}\mathrm{e}^{-t\hat{A}} \tag{0.1.2}$$

と定義する. $f(t)$ を $t=0$ の周りで展開することを考えると,

$$f(t) = f(0) + \frac{1}{1!}\left(\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{t=0}\right)t + \frac{1}{2!}\left(\left.\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right|_{t=0}\right)t^2 + \cdots \tag{0.1.3}$$

と書ける. さて,

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \hat{A}\mathrm{e}^{t\hat{A}}\hat{B}\mathrm{e}^{-t\hat{A}} - \mathrm{e}^{t\hat{A}}\hat{B}\hat{A}\mathrm{e}^{-t\hat{A}} \tag{0.1.4}$$

$$= \mathrm{e}^{t\hat{A}}\hat{A}\hat{B}\mathrm{e}^{-t\hat{A}} - \mathrm{e}^{t\hat{A}}\hat{B}\hat{A}\mathrm{e}^{-t\hat{A}} \tag{0.1.5}$$

$$= \mathrm{e}^{t\hat{A}}\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)\mathrm{e}^{-t\hat{A}} \tag{0.1.6}$$

$$= \mathrm{e}^{t\hat{A}}\left[\hat{A},\hat{B}\right]\mathrm{e}^{-t\hat{A}} \tag{0.1.7}$$

である. よって,

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{t=0} = \left[\hat{A},\hat{B}\right] \tag{0.1.8}$$

である. 2 階以上の微分では, **式** (0.1.7) において, $\hat{B} \to \left[\hat{A},\hat{B}\right]$ とすればよい. よって, **式** (0.1.3) に**式** (0.1.7) を代入すると,

$$f(t) = B + \left[\hat{A},\hat{B}\right]t + \frac{1}{2!}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]t^2 + \cdots \tag{0.1.9}$$

である. $t=1$ とすれば,

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right] + \frac{1}{2!}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] + \cdots \tag{0.1.10}$$

となる. 特に,

$$\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] = 0 \tag{0.1.11}$$

のとき,

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right] \tag{0.1.12}$$

である. □

0.2 Baker-Campbell-Hausdorff の公式 2

$$\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} = \exp\left(\hat{A} + \hat{B} + \frac{1}{2}\left[\hat{A},\hat{B}\right] + \frac{1}{12}\left[\left(\hat{A}-\hat{B}\right),\left[\hat{A},\hat{B}\right]\right] + \cdots\right) \tag{0.2.1}$$

なる式を示す.

Proof. $f(t)$ と $g(t)$ を，

$$\begin{cases} f(t) \coloneqq \mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}} = \mathrm{e}^{g(t)} \\ g(t) \coloneqq \log\left(\mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}}\right) = \log\left(f(t)\right) \end{cases} \tag{0.2.2}$$

と定義する．$f(t)$ の Taylor 展開を考える．

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}f(t) &= \hat{A}\mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}} + \mathrm{e}^{t\hat{A}}B\mathrm{e}^{t\hat{B}} && (0.2.3)\\
&= \mathrm{e}^{t\hat{A}}\left(\hat{A}+\hat{B}\right)\mathrm{e}^{t\hat{B}} && (0.2.4)\\
\frac{\mathrm{d}^2}{\mathrm{d}t^2}f(t) &= \mathrm{e}^{t\hat{A}}\left\{\hat{A}\left(\hat{A}+\hat{B}\right) + \left(\hat{A}+\hat{B}\right)\hat{B}\right\}\mathrm{e}^{t\hat{B}} && (0.2.5)\\
&= \mathrm{e}^{t\hat{A}}\left\{\hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2\right\}\mathrm{e}^{t\hat{B}} && (0.2.6)\\
&= \mathrm{e}^{t\hat{A}}\left\{\hat{A}^2 + \hat{A}\hat{B} + \hat{B}\hat{A} + \hat{B}^2 + \hat{A}\hat{B} - \hat{B}\hat{A}\right\}\mathrm{e}^{t\hat{B}} && (0.2.7)\\
&= \mathrm{e}^{t\hat{A}}\left\{\left(\hat{A}+\hat{B}\right)^2 + \left[\hat{A},\hat{B}\right]\right\}\mathrm{e}^{t\hat{B}} && (0.2.8)\\
\frac{\mathrm{d}^3}{\mathrm{d}t^3}f(t) &= \mathrm{e}^{t\hat{A}}\left\{\hat{A}\left(\hat{A} + 2\hat{A}\hat{B} + \hat{B}^2\right) + \left(\hat{A} + 2\hat{A}\hat{B} + \hat{B}^2\right)\hat{B}\right\}\mathrm{e}^{t\hat{B}} && (0.2.9)\\
&= \mathrm{e}^{t\hat{A}}\left\{\hat{A}^3 + 3\hat{A}^2\hat{B} + 3\hat{A}\hat{B}^2 + \hat{B}^3\right\}\mathrm{e}^{t\hat{B}} && (0.2.10)\\
&= \mathrm{e}^{t\hat{A}}\left\{\hat{A}^3 + \hat{A}^2\hat{B} + \hat{A}\hat{B}\hat{A} + \hat{B}\hat{A}^2 + \hat{B}^2\hat{A} + \hat{B}\hat{A}\hat{B} + \hat{A}\hat{B}^2 + \hat{B}^3 + 2\hat{A}^2\hat{B} - \hat{A}\hat{B}\hat{A} - \hat{B}\hat{A}^2 - \hat{B}^2\hat{A} - \hat{B}\hat{A}\hat{B} + 2\hat{A}\hat{B}^2\right\}\mathrm{e}^{t\hat{B}} && (0.2.11)\\
&= \mathrm{e}^{t\hat{A}}\left\{\left(\hat{A}+\hat{B}\right)^3 + \hat{A}^2\hat{B} - \hat{A}\hat{B}\hat{A} + \hat{A}^2\hat{B} - \hat{B}\hat{A}^2 + \hat{A}\hat{B}^2 - \hat{B}^2\hat{A} + \hat{A}\hat{B}^2 - \hat{B}\hat{A}\hat{B}\right\}\mathrm{e}^{t\hat{B}} && (0.2.12)\\
&= \mathrm{e}^{t\hat{A}}\left\{\left(\hat{A}+\hat{B}\right)^3 + \hat{A}\left[\hat{A},\hat{B}\right] + \left[\hat{A}^2,\hat{B}\right] + \left[\hat{A},\hat{B}^2\right] + \left[\hat{A},\hat{B}\right]\hat{B}\right\}\mathrm{e}^{t\hat{B}} && (0.2.13)
\end{aligned}$$

となる．$t=0$ 周りで $f(t)$ を Taylor 展開すると，

$$\begin{aligned}
f(t) &= f(0) + \frac{1}{1!}\left(\frac{\mathrm{d}}{\mathrm{d}t}f(t)\bigg|_{t=0}\right)t + \frac{1}{2!}\left(\frac{\mathrm{d}^2}{\mathrm{d}t^2}f(t)\bigg|_{t=0}\right)t^2 + \frac{1}{3!}\left(\frac{\mathrm{d}^3}{\mathrm{d}t^3}f(t)\bigg|_{t=0}\right)t^3 + \cdots && (0.2.14)\\
&= 1 + \frac{1}{1!}\left(\hat{A}+\hat{B}\right)t + \frac{1}{2!}\left\{\left(\hat{A}+\hat{B}\right)^2 + \left[\hat{A},\hat{B}\right]\right\}t^2 + \frac{1}{3!}\left\{\left(\hat{A}+\hat{B}\right)^3 + \hat{A}\left[\hat{A},\hat{B}\right] + \left[\hat{A}^2,\hat{B}\right] + \left[\hat{A},\hat{B}^2\right] + \left[\hat{A},\hat{B}\right]\hat{B}\right\}t^3 + \cdots && (0.2.15)\\
&= 1 + \hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3 + \cdots && (0.2.16)\\
& && (0.2.17)
\end{aligned}$$

と書ける．ただし，

$$\begin{aligned}
\hat{P}_1 &\coloneqq \frac{1}{1!}\left(\hat{A}+\hat{B}\right) && (0.2.18)\\
\hat{P}_2 &\coloneqq \frac{1}{2!}\left\{\left(\hat{A}+\hat{B}\right)^2 + \left[\hat{A},\hat{B}\right]\right\} && (0.2.19)\\
\hat{P}_3 &\coloneqq \frac{1}{3!}\left\{\left(\hat{A}+\hat{B}\right)^3 + \hat{A}\left[\hat{A},\hat{B}\right] + \left[\hat{A}^2,\hat{B}\right] + \left[\hat{A},\hat{B}^2\right] + \left[\hat{A},\hat{B}\right]\hat{B}\right\} && (0.2.20)
\end{aligned}$$

と定義した．$F(t)$ を，

$$\begin{aligned}
F(t) &\coloneqq f(t) - 1 && (0.2.21)\\
&= \hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3 + \cdots && (0.2.22)
\end{aligned}$$

と定義する．$h(x) \coloneqq \log(1+x)$ は $x=0$ のまわりで，

$$
\begin{aligned}
h(x) &= h(0) + \frac{1}{1!}\left(\frac{\mathrm{d}}{\mathrm{d}x}h(x)\bigg|_{x=0}\right)x + \frac{1}{2!}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}h(x)\bigg|_{x=0}\right)x^2 + \frac{1}{3!}\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}h(x)\bigg|_{x=0}\right)x^3 + \cdots && (0.2.23)\\
&= 0 + \frac{1}{1!}\frac{1}{1+0}x + \frac{1}{2!}\left(-\frac{1}{(1+0)^2}\right)x^2 + \frac{1}{3!}\left(\frac{2}{(1+0)^3}\right)x^3 + \cdots && (0.2.24)\\
&= x - \frac{x^2}{2} + \frac{x^3}{3} - \cdots && (0.2.25)
\end{aligned}
$$

であることと，$t \to 0$ で $F(t) \to 0$ であることを用いて $g(t)$ を $t=0$ の周りで Taylor 展開すると，

$$
\begin{aligned}
g(t) &= \log(f(t)) && (0.2.26)\\
&= \log(1+F(t)) && (0.2.27)\\
&= F(t) - \frac{F(t)^2}{2} + \frac{F(t)^3}{3} - \cdots && (0.2.28)\\
&= \left(\hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3\right) - \frac{1}{2}\left(\hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3\right)^2 + \frac{1}{3}\left(\hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3\right)^3 - \cdots && (0.2.29)\\
&= \hat{P}_1 t + \left(\hat{P}_2 - \frac{1}{2}\hat{P}_1^2\right)t^2 + \left\{\hat{P}_3 - \frac{1}{2}\left(\hat{P}_1\hat{P}_2 + \hat{P}_2\hat{P}_1\right) + \frac{1}{3}\hat{P}_1^3\right\}t^3 - \cdots && (0.2.30)
\end{aligned}
$$

となる．$\hat{P}_1$，$\hat{P}_2$，$\hat{P}_3$ の定義を思い出せば，

$$
\begin{aligned}
\left(t^1\text{の係数}\right) &= \hat{P}_1 = \hat{A} + \hat{B} && (0.2.31)\\
\left(t^2\text{の係数}\right) &= \hat{P}_2 - \frac{1}{2}\hat{P}_1^2 && (0.2.32)\\
&= \frac{1}{2}\left\{\left(\hat{A}+\hat{B}\right)^2 + \left[\hat{A},\hat{B}\right]\right\} - \frac{1}{2}\left(\hat{A}+\hat{B}\right)^2 && (0.2.33)\\
&= \frac{1}{2}\left[\hat{A},\hat{B}\right] && (0.2.34)\\
\left(t^3\text{の係数}\right) &= \hat{P}_3 - \frac{1}{2}\left(\hat{P}_1\hat{P}_2 + \hat{P}_2\hat{P}_1\right) + \frac{1}{3}\hat{P}_1^3 && (0.2.35)\\
&= \frac{1}{3!}\left\{\left(\hat{A}+\hat{B}\right)^3 + \hat{A}\left[\hat{A},\hat{B}\right] + \left[\hat{A}^2,\hat{B}\right] + \left[\hat{A},\hat{B}^2\right] + \left[\hat{A},\hat{B}\right]\hat{B}\right\}\\
&\quad - \frac{1}{2}\left[\left(\hat{A}+\hat{B}\right)\frac{1}{2!}\left\{\left(\hat{A}+\hat{B}\right)^2 + \left[\hat{A},\hat{B}\right]\right\} + \frac{1}{2!}\left\{\left(\hat{A}+\hat{B}\right)^2 + \left[\hat{A},\hat{B}\right]\right\}\left(\hat{A}+\hat{B}\right)\right]\\
&\quad + \frac{1}{3}\left(\hat{A}+\hat{B}\right)^3 && (0.2.36)\\
&= \frac{1}{6}\left(\hat{A}+\hat{B}\right)^3 + \frac{1}{6}\hat{A}\left[\hat{A},\hat{B}\right] + \frac{1}{6}\left\{\hat{A}\left[\hat{A},\hat{B}\right] + \left[\hat{A},\hat{B}\right]\hat{A}\right\} + \frac{1}{6}\left\{\hat{B}\left[\hat{A},\hat{B}\right] + \left[\hat{A},\hat{B}\right]\hat{B}\right\} + \frac{1}{6}\left[\hat{A},\hat{B}\right]\hat{B}\\
&\quad - \frac{1}{2}\left(\hat{A}+\hat{B}\right)^3 - \frac{1}{4}\hat{A}\left[\hat{A},\hat{B}\right] - \frac{1}{4}\hat{B}\left[\hat{A},\hat{B}\right] - \frac{1}{4}\left[\hat{A},\hat{B}\right]\hat{A} - \frac{1}{4}\left[\hat{A},\hat{B}\right]\hat{B}\\
&\quad + \frac{1}{3}\left(\hat{A}+\hat{B}\right)^3 && (0.2.37)\\
&= \frac{1}{12}\hat{A}\left[\hat{A},\hat{B}\right] - \frac{1}{12}\hat{B}\left[\hat{A},\hat{B}\right] + \frac{1}{12}\left[\hat{A},\hat{B}\right]\hat{A} - \frac{1}{12}\left[\hat{A},\hat{B}\right]\hat{B} && (0.2.38)\\
&= \frac{1}{12}\left(\hat{A}-\hat{B}\right)\left[\hat{A},\hat{B}\right] - \frac{1}{12}\left[\hat{A},\hat{B}\right]\left(\hat{A}-\hat{B}\right) && (0.2.39)\\
&= \frac{1}{12}\left[\left(\hat{A}-\hat{B}\right),\left[\hat{A},\hat{B}\right]\right] && (0.2.40)
\end{aligned}
$$

よって，

$$
\begin{aligned}
\mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}} &= f(t) = \mathrm{e}^{g(t)} && (0.2.41)\\
&= \exp\left\{\left(\hat{A}+\hat{B}\right)t + \frac{1}{2}\left[\hat{A},\hat{B}\right]t^2 + \frac{1}{12}\left[\left(\hat{A}-\hat{B}\right),\left[\hat{A},\hat{B}\right]\right]t^3 + \cdots\right\} && (0.2.42)
\end{aligned}
$$

(0.2.43)

となるから，$t=0$ とすれば，

$$e^{\hat{A}}e^{\hat{B}} = \exp\left\{\left(\hat{A}+\hat{B}\right)+\frac{1}{2}\left[\hat{A},\hat{B}\right]+\frac{1}{12}\left[\left(\hat{A}-\hat{B}\right),\left[\hat{A},\hat{B}\right]\right]+\cdots\right\} \tag{0.2.44}$$

となる．特に，

$$\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]=\left[\hat{B},\left[\hat{A},\hat{B}\right]\right]=0 \tag{0.2.45}$$

のときは，

$$e^{\hat{A}}e^{\hat{B}} = \exp\left\{\left(\hat{A}+\hat{B}\right)+\frac{1}{2}\left[\hat{A},\hat{B}\right]\right\} \tag{0.2.46}$$

となる． □