0.1 Baker-Campbell-Hausdorffの公式1

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

なる式を示す.

Proof. 函数 f(t) を,

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

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,

$$f(t) = f(0) + \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{t=0} t + \frac{1}{2!} \frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\Big|_{t=0} t^2 + \dots$$
 (0.1.3)

と書ける. さて,

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

$$(0.1.4)$$

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

$$(0.1.5)$$

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

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

である. よって,

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

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

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

である. t=1とすれば,

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

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

である.

0.2 Baker-Campbell-Hausdorffの公式 2

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

なる式を示す.

Proof. $f(t) \geq g(t) \geq 0$,

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

と定義する. f(t) の Taylor 展開を考える.

$$\frac{\mathrm{d}}{\mathrm{d}t}f(t) = \hat{A}\mathrm{e}^{t\hat{A}}\mathrm{e}^{t\hat{B}} + \mathrm{e}^{t\hat{A}}B\mathrm{e}^{t\hat{B}} \tag{0.2.3}$$

$$= e^{t\hat{A}} \left(\hat{A} + \hat{B} \right) e^{t\hat{B}} \tag{0.2.4}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}f(t) = \mathrm{e}^{t\hat{A}}\left\{\hat{A}\left(\hat{A}+\hat{B}\right) + \left(\hat{A}+\hat{B}\right)\hat{B}\right\}\mathrm{e}^{t\hat{B}} \tag{0.2.5}$$

$$= e^{t\hat{A}} \left\{ \hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2 \right\} e^{t\hat{B}}$$
 (0.2.6)

$$= e^{t\hat{A}} \left\{ \hat{A}^2 + \hat{A}\hat{B} + \hat{B}\hat{A} + \hat{B}^2 + \hat{A}\hat{B} - \hat{B}\hat{A} \right\} e^{t\hat{B}}$$
(0.2.7)

$$= e^{t\hat{A}} \left\{ \left(\hat{A} + \hat{B} \right)^2 + \left[\hat{A}, \hat{B} \right] \right\} e^{t\hat{B}} \tag{0.2.8}$$

$$\frac{d^3}{dt^3}f(t) = e^{t\hat{A}} \left\{ \hat{A} \left(\hat{A} + 2\hat{A}\hat{B} + \hat{B}^2 \right) + \left(\hat{A} + 2\hat{A}\hat{B} + \hat{B}^2 \right) \hat{B} \right\} e^{t\hat{B}}$$
(0.2.9)

$$= e^{t\hat{A}} \left\{ \hat{A}^3 + 3\hat{A}^2\hat{B} + 3\hat{A}\hat{B}^2 + \hat{B}^3 \right\} e^{t\hat{B}}$$
(0.2.10)

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

$$(0.2.11)$$

$$= e^{t\hat{A}} \left\{ \left(\hat{A} + \hat{B} \right)^3 + \hat{A}^2 \hat{B} - \hat{A} \hat{B} \hat{A} + \hat{A}^2 \hat{B} - \hat{B} \hat{A}^2 + \hat{A} \hat{B}^2 - \hat{B}^2 \hat{A} + \hat{A} \hat{B}^2 - \hat{B} \hat{A} \hat{B} \right\} e^{t\hat{B}}$$
(0.2.12)

$$= e^{t\hat{A}} \left\{ \left(\hat{A} + \hat{B} \right)^3 + \hat{A} \left[\hat{A}, \hat{B} \right] + \left[\hat{A}^2, \hat{B} \right] + \left[\hat{A}, \hat{B}^2 \right] + \left[\hat{A}, \hat{B} \right] \hat{B} \right\} e^{t\hat{B}}$$
(0.2.13)

となる. t = 0 周りで f(t) を Taylor 展開すると,

$$f(t) = f(0) + \frac{1}{1!} \frac{\mathrm{d}}{\mathrm{d}t} f(t) \Big|_{t=0} t + \frac{1}{2!} \frac{\mathrm{d}^2}{\mathrm{d}t^2} f(t) \Big|_{t=0} t^2 + \frac{1}{3!} \frac{\mathrm{d}^3}{\mathrm{d}t^3} f(t) \Big|_{t=0} t^3 + \cdots$$

$$(0.2.14)$$

$$=1+\frac{1}{1!}(\hat{A}+\hat{B})t+\frac{1}{2!}\{(\hat{A}+\hat{B})^{2}+[\hat{A},\hat{B}]\}t^{2}+\frac{1}{3!}\{(\hat{A}+\hat{B})^{3}+\hat{A}[\hat{A},\hat{B}]+[\hat{A}^{2},\hat{B}]+[\hat{A},\hat{B}^{2}]+[\hat{A},\hat{B}]\hat{B}\}t^{3}+\cdots$$
(0.2.15)

$$=1+\hat{P}_1t+\hat{P}_2t^2+\hat{P}_3t^3+\cdots \tag{0.2.16}$$

(0.2.17)

と書ける. ただし,

$$\hat{P}_1 := \frac{1}{1!} (\hat{A} + \hat{B})$$
 (0.2.18)

$$\hat{P}_2 := \frac{1}{2!} \left\{ \left(\hat{A} + \hat{B} \right)^2 + \left[\hat{A}, \hat{B} \right] \right\} \tag{0.2.19}$$

$$\hat{P}_{3} := \frac{1}{3!} \left\{ \left(\hat{A} + \hat{B} \right)^{3} + \hat{A} \left[\hat{A}, \hat{B} \right] + \left[\hat{A}^{2}, \hat{B} \right] + \left[\hat{A}, \hat{B}^{2} \right] + \left[\hat{A}, \hat{B} \right] \hat{B} \right\}$$
(0.2.20)

と定義した. F(t) を,

$$F(t) := f(t) - 1 \tag{0.2.21}$$

$$= \hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3 + \cdots$$
 (0.2.22)

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

$$h(x) = h(0) + \frac{1}{1!} \left(\frac{\mathrm{d}}{\mathrm{d}x} h(x) \Big|_{x=0} \right) x + \frac{1}{2!} \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} h(x) \Big|_{x=0} \right) x^2 + \frac{1}{3!} \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3} h(x) \Big|_{x=0} \right) x^3 + \dots$$
 (0.2.23)

$$= 0 + \frac{1}{1!} \frac{1}{1+0} x + \frac{1}{2!} \left(-\frac{1}{(1+0)^2} \right) x^2 + \frac{1}{3!} \left(\frac{2}{(1+0)^3} \right) x^3 + \dots$$
 (0.2.24)

$$=x-\frac{x^2}{2}+\frac{x^3}{3}+\cdots ag{0.2.25}$$

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,

$$g(t) = \log(f(t)) \tag{0.2.26}$$

$$= \log(1 + F(t)) \tag{0.2.27}$$

$$= F(t) - \frac{F(t)^2}{2} + \frac{F(t)^3}{3} - \dots$$
 (0.2.28)

$$= \left(\hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3\right) - \frac{1}{2} \left(\hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3\right)^2 + \frac{1}{3} \left(\hat{P}_1 t + \hat{P}_2 t^2 + \hat{P}_3 t^3\right)^3 - \dots$$
 (0.2.29)

$$= \hat{P}_1 t + \left(\hat{P}_2 - \frac{1}{2}\hat{P}_1^2\right) t^2 + \left\{\hat{P}_3 - \frac{1}{2}\left(\hat{P}_1\hat{P}_2 + \hat{P}_2\hat{P}_1\right) + \frac{1}{3}\hat{P}_1^3\right\} t^3 - \dots$$
 (0.2.30)

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

$$(t^1 \mathcal{O}$$
係数 $) = \hat{P}_1 = \hat{A} + \hat{B}$ (0.2.31)

$$(t^2 \mathcal{O}(条数) = \hat{P}_2 - \frac{1}{2}\hat{P}_1^2 \tag{0.2.32}$$

$$= \frac{1}{2} \left\{ \left(\hat{A} + \hat{B} \right)^2 + \left[\hat{A}, \hat{B} \right] \right\} - \frac{1}{2} \left(\hat{A} + \hat{B} \right)^2 \tag{0.2.33}$$

$$=\frac{1}{2}\left[\hat{A},\hat{B}\right] \tag{0.2.34}$$

$$(t^{3} \mathcal{O} 係数) = \hat{P}_{3} - \frac{1}{2} \left(\hat{P}_{1} \hat{P}_{2} + \hat{P}_{2} \hat{P}_{1} \right) + \frac{1}{3} \hat{P}_{1}^{3}$$

$$= \frac{1}{3!} \left\{ \left(\hat{A} + \hat{B} \right)^{3} + \hat{A} \left[\hat{A}, \hat{B} \right] + \left[\hat{A}^{2}, \hat{B} \right] + \left[\hat{A}, \hat{B}^{2} \right] + \left[\hat{A}, \hat{B} \right] \hat{B} \right\}$$

$$- \frac{1}{2} \left[\left(\hat{A} + \hat{B} \right) \frac{1}{2!} \left\{ \left(\hat{A} + \hat{B} \right)^{2} + \left[\hat{A}, \hat{B} \right] \right\} + \frac{1}{2!} \left\{ \left(\hat{A} + \hat{B} \right)^{2} + \left[\hat{A}, \hat{B} \right] \right\} \left(\hat{A} + \hat{B} \right) \right]$$

$$+ \frac{1}{3} \left(\hat{A} + \hat{B} \right)^{3}$$

$$= \frac{1}{6} \left(\hat{A} + \hat{B} \right)^{3} + \frac{1}{6} \hat{A} \left[\hat{A}, \hat{B} \right] + \frac{1}{6} \left\{ \hat{A} \left[\hat{A}, \hat{B} \right] + \left[\hat{A}, \hat{B} \right] \hat{A} \right\} + \frac{1}{6} \left\{ \hat{B} \left[\hat{A}, \hat{B} \right] + \left[\hat{A}, \hat{B} \right] \hat{B} \right\}$$

$$- \frac{1}{2} \left(\hat{A} + \hat{B} \right)^{3} - \frac{1}{4} \hat{A} \left[\hat{A}, \hat{B} \right] - \frac{1}{4} \hat{B} \left[\hat{A}, \hat{B} \right] - \frac{1}{4} \left[\hat{A}, \hat{B} \right] \hat{A} - \frac{1}{4} \left[\hat{A}, \hat{B} \right] \hat{B}$$

$$- \frac{1}{2} \left(\hat{A} + \hat{B} \right)^{3} - \frac{1}{4} \hat{A} \left[\hat{A}, \hat{B} \right] - \frac{1}{4} \hat{B} \left[\hat{A}, \hat{B} \right] - \frac{1}{4} \left[\hat{A}, \hat{B} \right] \hat{A} - \frac{1}{4} \left[\hat{A}, \hat{B} \right] \hat{B}$$

$$+\frac{1}{3}(\hat{A}+\hat{B})^3$$
 (0.2.37)

$$= \frac{1}{12}\hat{A}[\hat{A}, \hat{B}] - \frac{1}{12}\hat{B}[\hat{A}, \hat{B}] + \frac{1}{12}[\hat{A}, \hat{B}]\hat{A} - \frac{1}{12}[\hat{A}, \hat{B}]\hat{B}$$
(0.2.38)

$$= \frac{1}{12} (\hat{A} - \hat{B}) [\hat{A}, \hat{B}] - \frac{1}{12} [\hat{A}, \hat{B}] (\hat{A} - \hat{B})$$
(0.2.39)

$$=\frac{1}{12}\left[\left(\hat{A}-\hat{B}\right),\left[\hat{A},\hat{B}\right]\right] \tag{0.2.40}$$

よって,

$$e^{t\hat{A}}e^{t\hat{B}} = f(t) = e^{g(t)}$$
 (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)

(0.2.43)

となるから, t=0とすれば,

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

となる. 特に,

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

$$\iff \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] = \left[\hat{B}, \left[\hat{A}, \hat{B}\right]\right] = 0 \tag{0.2.46}$$

のときは,

$$e^{\hat{A}}e^{\hat{B}} = \exp\left\{ \left(\hat{A} + \hat{B} \right) + \frac{1}{2} \left[\hat{A}, \hat{B} \right] \right\}$$
 (0.2.47)