

Commutation relation related to the mirror-reflection operator based on Baker-Hausdorff lemma

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Here we discuss the property of the mirror-reflection operator, \hat{M}_y , which is defined by the product of rotation operator \hat{Y} (with rotation angle $\theta = \pi$) and the parity operator, $\hat{\pi}$,

$$\hat{M}_y = \hat{Y}\hat{\pi}.$$

where $\hat{Y} = \exp(-\frac{i}{\hbar}\pi\hat{J}_y)$. To this end, we will evaluate a operator $\hat{M}_y^{-1}\hat{A}\hat{M}_y$, where \hat{A} is an operator such as the position vector, momentum, and angular momentum, using the Baker-Hausdorff lemma. We are interested in the case of positive integer of the angular momentum

1. Baker-Hausdorff lemma

To calculate these operators, we use the Baker-Hausdorff lemma,

$$\begin{aligned} \exp(i\lambda\hat{G})\hat{A}\exp(-i\lambda\hat{G}) &= \hat{A} + \frac{(i\lambda)}{1!}[\hat{G}, \hat{A}] + \frac{(i\lambda)^2}{2!}[\hat{G}, [\hat{G}, \hat{A}]] + \frac{(i\lambda)^3}{3!}[\hat{G}, [\hat{G}, [\hat{G}, \hat{A}]]] \\ &+ \frac{(i\lambda)^4}{4!}[\hat{G}, [\hat{G}, [\hat{G}, [\hat{G}, \hat{A}]]]] + \dots \end{aligned}$$

where \hat{G} is a Hermitian operator and λ is a real parameter. Using the commutation relations

$$[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z, \quad [\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x, \quad [\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y$$

we obtain

$$\begin{aligned}
\exp\left(\frac{i\alpha}{\hbar}\hat{J}_z\right)\hat{J}_x\exp\left(-\frac{i\alpha}{\hbar}\hat{J}_z\right) &= \hat{J}_x + \frac{\left(\frac{i\alpha}{\hbar}\right)}{1!}[\hat{J}_z, \hat{J}_x] + \frac{\left(\frac{i\alpha}{\hbar}\right)^2}{2!}[\hat{J}_z, [\hat{J}_z, \hat{J}_x]] + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}[\hat{J}_z, [\hat{J}_z, [\hat{J}_z, \hat{J}_x]]] + \dots \\
&= \hat{J}_x + \frac{\left(\frac{i\alpha}{\hbar}\right)}{1!}(i\hbar\hat{J}_y) + \frac{\left(\frac{i\alpha}{\hbar}\right)^2}{2!}[\hat{J}_z, i\hbar\hat{J}_y] + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}[\hat{J}_z, [\hat{J}_z, i\hbar\hat{J}_y]] + \dots \\
&= \hat{J}_x - \alpha\hat{J}_y + \frac{\left(\frac{i\alpha}{\hbar}\right)^2}{2!}i\hbar(-i\hbar\hat{J}_x) + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}i\hbar(-i\hbar)[\hat{J}_z, \hat{J}_x] + \dots \\
&= \hat{J}_x - \alpha\hat{J}_y - \frac{\alpha^2}{2!}\hat{J}_x + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}\hbar^2(i\hbar)\hat{J}_y, + \dots \\
&= \hat{J}_x - \alpha\hat{J}_y - \frac{\alpha^2}{2!}\hat{J}_x + \frac{\alpha^3}{3!}\hat{J}_y, + \dots \\
&= \hat{J}_x\left(1 - \frac{\alpha^2}{2!} + \frac{\alpha^4}{4!} + \dots\right) - \left(\alpha - \frac{\alpha^3}{3!} + \frac{\alpha^5}{5!} + \dots\right)\hat{J}_y, \\
&= \hat{J}_x \cos \alpha - \hat{J}_y \sin \alpha
\end{aligned}$$

The results of the calculations which are obtained in a similar way, are summarized as follows.

$$\exp\left(\frac{i}{\hbar}\alpha\hat{J}_z\right)\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix}\exp\left(-\frac{i}{\hbar}\alpha\hat{J}_z\right) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix} = \mathfrak{R}_z(\alpha)\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix},$$

$$\exp\left(\frac{i}{\hbar}\alpha\hat{J}_x\right)\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix}\exp\left(-\frac{i}{\hbar}\alpha\hat{J}_x\right) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & -\sin \alpha \\ 0 & \sin \alpha & \cos \alpha \end{pmatrix}\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix} = \mathfrak{R}_x(\alpha)\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix},$$

$$\exp\left(\frac{i}{\hbar}\alpha\hat{J}_y\right)\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix}\exp\left(-\frac{i}{\hbar}\alpha\hat{J}_y\right) = \begin{pmatrix} \cos \alpha & 0 & \sin \alpha \\ 0 & 1 & 0 \\ -\sin \alpha & 0 & \cos \alpha \end{pmatrix}\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix} = \mathfrak{R}_y(\alpha)\begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix},$$

where $\mathfrak{R}_x(\alpha)$, $\mathfrak{R}_y(\alpha)$, and $\mathfrak{R}_z(\alpha)$ are the rotation matrices.

2. Evaluation of $\hat{M}_y^{-1}\hat{A}\hat{M}_y$

Here we consider the orbital angular momentum \hat{L}_x , \hat{L}_y , and \hat{L}_z ($j = l$, a positive integer). The following commutation relations are obtained.

$$[\hat{x}, \hat{L}_x] = 0, \quad [\hat{x}, \hat{L}_y] = i\hbar\hat{z}, \quad [\hat{x}, \hat{L}_z] = -i\hbar\hat{y},$$

$$[\hat{y}, \hat{L}_x] = -i\hbar\hat{z}, \quad [\hat{y}, \hat{L}_y] = 0, \quad [\hat{y}, \hat{L}_z] = i\hbar\hat{x},$$

$$[\hat{z}, \hat{L}_x] = i\hbar\hat{y}, \quad [\hat{z}, \hat{L}_y] = i\hbar\hat{x}, \quad [\hat{z}, \hat{L}_z] = 0,$$

$$[\hat{p}_x, \hat{L}_x] = 0, \quad [\hat{p}_x, \hat{L}_y] = i\hbar\hat{p}_z, \quad [\hat{p}_x, \hat{L}_z] = -i\hbar\hat{p}_y,$$

$$[\hat{p}_y, \hat{L}_x] = -i\hbar\hat{p}_z, \quad [\hat{p}_y, \hat{L}_y] = 0, \quad [\hat{p}_y, \hat{L}_z] = i\hbar\hat{p}_x,$$

$$[\hat{p}_z, \hat{L}_x] = i\hbar\hat{p}_y, \quad [\hat{p}_z, \hat{L}_y] = -i\hbar\hat{p}_x, \quad [\hat{p}_z, \hat{L}_z] = 0,$$

These commutation relations can be expressed as

$$[\hat{L}_y, \hat{A}_x] = -i\hbar\hat{A}_z, \quad [\hat{L}_y, \hat{A}_z] = i\hbar\hat{A}_x,$$

or

$$[\hat{A}_x, \hat{L}_y] = i\hbar\hat{A}_z, \quad [\hat{A}_z, \hat{L}_y] = -i\hbar\hat{A}_x,$$

where $\hat{A} = \hat{r}$, and $\hat{A} = \hat{p}$. Using these commutation relations and the Baker-Hausdorff lemma, we have

$$\begin{aligned}
\exp\left(\frac{i\alpha}{\hbar}\hat{L}_y\right)\hat{A}_x\exp\left(-\frac{i\alpha}{\hbar}\hat{L}_y\right) &= \hat{A}_x + \frac{\left(\frac{i\alpha}{\hbar}\right)}{1!}[\hat{L}_y, \hat{A}_x] + \frac{\left(\frac{i\alpha}{\hbar}\right)^2}{2!}[\hat{L}_y, [\hat{L}_y, \hat{A}_x]] + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}[\hat{L}_y, [\hat{L}_y, [\hat{L}_y, \hat{A}_x]]] + \dots \\
&= \hat{A}_x + \frac{\left(\frac{i\alpha}{\hbar}\right)}{1!}(-i\hbar\hat{A}_z) + \frac{\left(\frac{i\alpha}{\hbar}\right)^2}{2!}[\hat{L}_y, -i\hbar\hat{A}_z] + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}[\hat{L}_y, [\hat{L}_y, -i\hbar\hat{A}_z]] + \dots \\
&= \hat{A}_x + \alpha\hat{A}_z + \frac{\left(\frac{i\alpha}{\hbar}\right)^2}{2!}(-i\hbar)i\hbar\hat{A}_x + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}(-i\hbar)(i\hbar)[\hat{L}_y, \hat{A}_x] + \dots \\
&= \hat{A}_x + \alpha\hat{A}_z + \frac{\left(\frac{i\alpha}{\hbar}\right)^2}{2!}\hbar^2\hat{A}_x + \frac{\left(\frac{i\alpha}{\hbar}\right)^3}{3!}\hbar^2(-i\hbar)\hat{A}_z + \dots \\
&= \hat{A}_x + \alpha\hat{A}_z - \frac{1}{2!}\alpha^2\hat{A}_x - \frac{\alpha^3}{3!}\hat{A}_z + \dots \\
&= \hat{A}_x\left(1 - \frac{1}{2!}\alpha^2 + \frac{1}{4!}\alpha^4 \dots\right) + \hat{A}_z\left(\alpha - \frac{\alpha^3}{3!} + \frac{\alpha^5}{5!} \dots\right) \\
&= \hat{A}_x \cos \alpha + \hat{A}_z \sin \alpha
\end{aligned}$$

The results of the calculation are summarized as follows.

$$\exp\left(\frac{i}{\hbar}\alpha\hat{L}_z\right)\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix}\exp\left(-\frac{i}{\hbar}\alpha\hat{L}_z\right) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix} = \mathfrak{R}_z(\alpha)\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix},$$

$$\exp\left(\frac{i}{\hbar}\alpha\hat{L}_x\right)\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix}\exp\left(-\frac{i}{\hbar}\alpha\hat{L}_x\right) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & -\sin \alpha \\ 0 & \sin \alpha & \cos \alpha \end{pmatrix}\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix} = \mathfrak{R}_x(\alpha)\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix},$$

$$\exp\left(\frac{i}{\hbar}\alpha\hat{L}_y\right)\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix}\exp\left(-\frac{i}{\hbar}\alpha\hat{L}_y\right) = \begin{pmatrix} \cos \alpha & 0 & \sin \alpha \\ 0 & 1 & 0 \\ -\sin \alpha & 0 & \cos \alpha \end{pmatrix}\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix} = \mathfrak{R}_y(\alpha)\begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix}.$$

When $\alpha = \pi$, we assume that

$$\hat{Y} = \exp\left(-\frac{i}{\hbar}\alpha\hat{L}_y\right).$$

Then we get

$$Y^{-1} \begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix} \hat{Y} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \hat{A}_x \\ \hat{A}_y \\ \hat{A}_z \end{pmatrix}.$$

(i) $\hat{A} = \hat{r}$

$$Y^{-1} \hat{x} \hat{Y} = -\hat{x}, \quad Y^{-1} \hat{y} \hat{Y} = \hat{y}, \quad Y^{-1} \hat{z} \hat{Y} = -\hat{z}.$$

(ii) $\hat{A} = \hat{p}$

$$Y^{-1} \hat{p}_x \hat{Y} = -\hat{p}_x, \quad Y^{-1} \hat{p}_y \hat{Y} = \hat{p}_y, \quad Y^{-1} \hat{p}_z \hat{Y} = -\hat{p}_z.$$

Using the above relations we have

(a) $\hat{L}_x = \hat{y} \hat{p}_z - \hat{z} p_y$

$$\begin{aligned} \hat{Y}^{-1} \hat{L}_x \hat{Y} &= \hat{Y}^{-1} (\hat{y} \hat{p}_z - \hat{z} p_y) \hat{Y} \\ &= (\hat{Y}^{-1} \hat{y} \hat{Y}) (\hat{Y}^{-1} \hat{p}_z \hat{Y}) - (\hat{Y}^{-1} \hat{z} \hat{Y}) (\hat{Y}^{-1} \hat{p}_y \hat{Y}) \\ &= -(\hat{y} \hat{p}_z - \hat{z} \hat{p}_y) \\ &= -\hat{L}_x \end{aligned}$$

(b) $\hat{L}_y = \hat{z} \hat{p}_x - \hat{x} \hat{p}_z$

$$\begin{aligned} \hat{Y}^{-1} \hat{L}_y \hat{Y} &= \hat{Y}^{-1} (\hat{z} \hat{p}_x - \hat{x} \hat{p}_z) \hat{Y} \\ &= (\hat{Y}^{-1} \hat{z} \hat{Y}) (\hat{Y}^{-1} \hat{p}_x \hat{Y}) - (\hat{Y}^{-1} \hat{x} \hat{Y}) (\hat{Y}^{-1} \hat{p}_z \hat{Y}) \\ &= \hat{z} \hat{p}_x - \hat{x} \hat{p}_z \\ &= \hat{L}_y \end{aligned}$$

(c) $\hat{L}_z = \hat{x} \hat{p}_y - \hat{y} \hat{p}_x$

$$\begin{aligned} \hat{Y}^{-1} \hat{L}_z \hat{Y} &= \hat{Y}^{-1} (\hat{x} \hat{p}_y - \hat{y} \hat{p}_x) \hat{Y} \\ &= (\hat{Y}^{-1} \hat{x} \hat{Y}) (\hat{Y}^{-1} \hat{p}_y \hat{Y}) - (\hat{Y}^{-1} \hat{y} \hat{Y}) (\hat{Y}^{-1} \hat{p}_x \hat{Y}) \\ &= -(\hat{x} \hat{p}_y - \hat{y} \hat{p}_x) \\ &= -\hat{L}_z \end{aligned}$$

3. Properties of mirror-reflection operator

Here we consider only the orbital angular momentum. The mirror-reflection operator \hat{M}_y is defined as

$$\hat{M}_y = \hat{Y}\hat{\pi} = \hat{\pi}\hat{Y}, \quad \hat{M}_y^{-1} = (\hat{Y}\hat{\pi})^{-1} = \hat{\pi}^{-1}\hat{Y}^{-1} = \hat{\pi}\hat{Y}^{-1},$$

for the mirror reflection at $y = 0$ plane (the z - x plane). $\hat{\pi}$ is the parity operator, where

$$\hat{\pi}^{-1} = \hat{\pi} = \hat{\pi}^+,$$

$$\hat{\pi}\hat{r}\hat{\pi} = -\hat{r}, \quad \hat{\pi}\hat{p}\hat{\pi} = -\hat{p}, \quad \hat{\pi}\hat{L}\hat{\pi} = \hat{L}$$

$$\hat{\pi}\hat{Y}\hat{\pi} = \hat{Y}.$$

We note that

$$\hat{M}_y^2 = \hat{Y}\hat{\pi}\hat{Y}\hat{\pi} = \hat{Y}^2 = \hat{1}.$$

Using the properties of \hat{Y} and $\hat{\pi}$, we get

$$\hat{M}_y^{-1}\hat{x}\hat{M}_y = \hat{\pi}(\hat{Y}^{-1}\hat{x}\hat{Y})\hat{\pi} = -\hat{\pi}\hat{x}\hat{\pi} = \hat{x},$$

$$\hat{M}_y^{-1}\hat{y}\hat{M}_y = \hat{\pi}(\hat{Y}^{-1}\hat{y}\hat{Y})\hat{\pi} = \hat{\pi}\hat{y}\hat{\pi} = -\hat{y},$$

$$\hat{M}_y^{-1}\hat{z}\hat{M}_y = \hat{\pi}(\hat{Y}^{-1}\hat{z}\hat{Y})\hat{\pi} = -\hat{\pi}\hat{z}\hat{\pi} = \hat{z}.$$

Similarly, for the momentum operator we have

$$\hat{M}_y^{-1}\hat{p}_x\hat{M}_y = \hat{\pi}(\hat{Y}^{-1}\hat{p}_x\hat{Y})\hat{\pi} = -\hat{\pi}\hat{p}_x\hat{\pi} = \hat{p}_x,$$

$$\hat{M}_y^{-1}\hat{p}_y\hat{M}_y = \hat{\pi}(\hat{Y}^{-1}\hat{p}_y\hat{Y})\hat{\pi} = \hat{\pi}\hat{p}_y\hat{\pi} = -\hat{p}_y,$$

$$\hat{M}_y^{-1}\hat{p}_z\hat{M}_y = \hat{\pi}(\hat{Y}^{-1}\hat{p}_z\hat{Y})\hat{\pi} = -\hat{\pi}\hat{p}_z\hat{\pi} = \hat{p}_z.$$

For the orbital angular momentum,

$$\hat{M}_y^{-1} \hat{L}_x \hat{M}_y = \hat{\pi} (\hat{Y}^{-1} \hat{L}_x \hat{Y}) \hat{\pi} = -\hat{L}_x,$$

$$\hat{M}_y^{-1} \hat{L}_y \hat{M}_y = \hat{L}_y,$$

$$\hat{M}_y^{-1} \hat{L}_z \hat{M}_y = -\hat{L}_z.$$

4. Selection rule for the matrix element

We define the matrix

$$A_{\beta\alpha} = \langle \beta | \hat{A} | \alpha \rangle.$$

We also assume that

$$\hat{M}_y | \alpha \rangle = \eta_\alpha | \alpha \rangle, \quad \hat{M}_y | \beta \rangle = \eta_\beta | \beta \rangle,$$

and

$$\hat{A}' = \hat{M}_y \hat{A} \hat{M}_y^{-1} = \eta_A \hat{A}.$$

When $\eta_A = 1$, \hat{A} is even and when $\eta_A = -1$, \hat{A} is odd. We now calculate the matrix element

$$\begin{aligned} A_{\beta\alpha} &= \langle \beta | \hat{A} | \alpha \rangle \\ &= \langle \beta | \hat{M}_y^{-1} \hat{M}_y \hat{A} \hat{M}_y^{-1} \hat{M}_y | \alpha \rangle \\ &= \langle \beta | \hat{M}_y^+ \hat{M}_y \hat{A} \hat{M}_y^{-1} \hat{M}_y | \alpha \rangle \\ &= \eta_\alpha \eta_\beta \eta_A \langle \beta | \hat{A} | \alpha \rangle \\ &= \eta_\alpha \eta_\beta \eta_A A_{\beta\alpha} \end{aligned}$$

When $\eta_\alpha \eta_\beta \eta_A = 1$, $A_{\beta\alpha} \neq 0$. When $\eta_\alpha \eta_\beta \eta_A = -1$, we have $A_{\beta\alpha} = 0$. Thus it is required that

$$\eta_\alpha \eta_\beta \eta_A = 1.$$

4. The condition for $\eta_\beta \eta_A$

$$\begin{aligned}\langle \beta | \alpha \rangle &= \langle \beta | \hat{M}_y^{-1} \hat{M}_y \hat{M}_y^{-1} \hat{M}_y | \alpha \rangle \\ &= \eta_\alpha \eta_\beta \langle \beta | \alpha \rangle\end{aligned}$$

If $\eta_\alpha \eta_\beta = -1$, $\langle \beta | \alpha \rangle = 0$. (orthogonal to each other)

If $\eta_\alpha \eta_\beta = 1$, $\langle \beta | \alpha \rangle \neq 0$. (not orthogonal to each other).

APPENDIX-I Baker-Hausdorff lemma

This is a very useful tool to disentangle exponentials of certain operators often appear in quantum mechanics. Suppose that \hat{A} and \hat{B} are two operators such that

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

where \hat{C} commutes with both \hat{A} and \hat{B} ;

$$[\hat{C}, \hat{A}] = 0, \quad [\hat{C}, \hat{B}] = 0.$$

Then the Baker-Hausdorff lemma holds:

$$\exp(\alpha \hat{A} + \beta \hat{B}) = \exp(\beta \hat{B}) \exp(\alpha \hat{A}) \exp\left(\frac{\alpha \beta}{2} \hat{C}\right)$$

((Proof))

We consider

$$\hat{F}(\alpha) = \exp(\alpha \hat{A} + \beta \hat{B})$$

which is a function of α only. The derivative of $\hat{F}(\alpha)$ with respect to α can be calculated using the definition of $\hat{F}(\alpha)$ in terms of its Taylor series expansion;

$$\hat{F}(\alpha) = \sum_{n=0}^{\infty} \frac{1}{n!} (\alpha \hat{A} + \beta \hat{B})^n$$

$$\begin{aligned}
\frac{d}{d\alpha} \hat{F}(\alpha) &= \sum_{n=0}^{\infty} \frac{1}{n!} \{ \hat{A}(\alpha\hat{A} + \beta\hat{B})^{n-1} + (\alpha\hat{A} + \beta\hat{B})\hat{A}(\alpha\hat{A} + \beta\hat{B})^{n-2} \\
&\quad + (\alpha\hat{A} + \beta\hat{B})^2 \hat{A}(\alpha\hat{A} + \beta\hat{B})^{n-3} + \dots + (\alpha\hat{A} + \beta\hat{B})^{n-1} \hat{A} \} \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \{ n(\alpha\hat{A} + \beta\hat{B})^{n-1} \hat{A} + (n-1)\beta\hat{C}(\alpha\hat{A} + \beta\hat{B})^{n-2} \\
&\quad + (n-2)\beta\hat{C}(\alpha\hat{A} + \beta\hat{B})^{n-2} + \dots + \beta\hat{C}(\alpha\hat{A} + \beta\hat{B})^{n-2} \} \\
&= \hat{F}A + \frac{\beta}{2} FC
\end{aligned}$$

Integrating this equation over α from 0 to α , we find that

$$\hat{F}(\alpha) = \hat{F}(\alpha=0) \exp\left(\alpha\hat{A} + \frac{\alpha\beta}{2}\hat{C}\right),$$

$$\hat{F}(\alpha=0) = \sum_{n=0}^{\infty} \frac{1}{n!} (\beta\hat{B})^n = \exp(\beta\hat{B})$$

where \hat{C} commutes with \hat{A} . Then we obtain

$$\hat{F}(\alpha) = \exp(\beta\hat{B}) \exp(\alpha\hat{A}) \exp\left(\frac{\alpha\beta}{2}\hat{C}\right)$$

APPENDIX II

K. Gottfried and T.-M. Yan, Quantum Mechanics: Fundamentals 2nd edition (Springer, 2003).

The Baker-Hausdorff lemma for arbitrary \hat{A} and \hat{B} ,

$$\exp(\hat{A})\exp(\hat{B}) = \exp\left(\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}([\hat{A}, [\hat{A}, \hat{B}]] - [\hat{B}, [\hat{A}, \hat{B}]]) + \dots\right).$$

If $\hat{C} = [\hat{A}, \hat{B}]$ commutes with both \hat{A} and \hat{B} ,

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

or

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

In order to prove this formula, we first can show that

$$[\hat{B}, \exp(x\hat{A})] = \exp(x\hat{A})[\hat{B}, \hat{A}]x.$$

Next we define

$$\hat{G}(x) = \exp(x\hat{A})\exp(x\hat{B})$$

And we can show that

$$\frac{d\hat{G}(x)}{dx} = (\hat{A} + \hat{B} + [\hat{A}, \hat{B}]x)\hat{G}$$

Integrate this to obtain

$$\hat{G}(x) = \exp(x\hat{A})\exp(x\hat{B}) = \exp\left\{(\hat{A} + \hat{B})x + \frac{1}{2}[\hat{A}, \hat{B}]x^2\right\}\hat{G}(x=0)$$

with

$$\hat{G}(x=0) = \hat{1}$$

Then we have for $x = 1$,

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