I.9 Functions of operators

Consider a function $f(x)$ (where $x \in \mathbb{R}$ or $x \in \mathbb{C}$) that can be written as a power series:

$$f(x) = \sum_{n=0}^{\infty} a_n x^n$$

We can define the same function of an operator $\hat{S}$ through the corresponding series

$$f(\hat{S}) = \sum_{n=0}^{\infty} a_n \hat{S}^n$$

This makes sense if the series somehow converges.

To see what this means, consider

$$e^{\hat{S}} = \sum_{n=0}^{\infty} \frac{\hat{S}^n}{n!}$$

Let us assume that $\hat{S}$ is Hermitian. By going to the eigenbasis of $\hat{S}$, it is represented by a diagonal matrix:

$$\hat{S} \leftrightarrow \begin{pmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{pmatrix}$$

Since from $\hat{S} |\omega_i\rangle = \omega_i |\omega_i\rangle$ it follows that $\hat{S}^m |\omega_i\rangle = \omega_i^m |\omega_i\rangle$,

$\hat{S}^m$ is represented by $\hat{S}^m = \begin{pmatrix} \omega_1^m & 0 & \cdots & 0 \\ 0 & \omega_2^m & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n^m \end{pmatrix}$ and $e^{\hat{S}}$ by

$$e^{\hat{S}} \leftrightarrow \begin{pmatrix} e^{\frac{\omega_1}{1!}} & 0 & \cdots & 0 \\ 0 & e^{\frac{\omega_2}{2!}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{\frac{\omega_n}{n!}} \end{pmatrix}$$
So \( f(\Omega) = \sum_{n=0}^{\infty} a_n \hat{\Omega}^n \) converges iff
\[ f(\omega_i) = \sum_{n=0}^{\infty} a_n \omega_i^n \] converges for all eigenvalues \( \omega_i \).

**Derivatives of operator w.r.t. parameters**

For an operator \( \hat{\Theta}(\lambda) \),
\[ \frac{d}{d\lambda} \Theta(\lambda) := \lim_{\Delta\lambda \to 0} \frac{\hat{\Theta}(\lambda + \Delta \lambda) - \hat{\Theta}(\lambda)}{\Delta \lambda} \]
(\( \lambda \in \mathbb{R} \) is a parameter)

Operationally, you express the operator through its matrix elements in some (\( \lambda \)-independent) basis and differentiate the matrix elements which are standard complex functions of \( \lambda \).

**Important example:**
\( \hat{\Theta}(\lambda) = e^{\lambda \hat{S}} \) with \( \hat{S} = \hat{S}^+ \)

By going to the eigenbasis of \( \hat{S} \) (where it is diagonal), one shows
\[ \frac{d}{d\lambda} \hat{\Theta}(\lambda) = \hat{S} e^{\lambda \hat{S}} = e^{\lambda \hat{S}} = \hat{\Theta}(\lambda) \hat{S} = \hat{S} \hat{\Theta}(\lambda) \]

If \( \hat{S} \) is not here then, look at the power series:
\[ \frac{d}{d\lambda} \sum_{n=0}^{\infty} \frac{\lambda^n \hat{S}^n}{n!} = \sum_{n=1}^{\infty} \frac{\lambda^{n-1} \hat{S}^n}{(n-1)!} = \hat{S} \sum_{n=1}^{\infty} \frac{\lambda^{n-1} \hat{S}^{n-1}}{(n-1)!} = \hat{S} e^{\lambda \hat{S}} \]

So the same holds true whenever the power series converges.

Conversely, the solution of the differential equation
\[ \frac{d}{d\lambda} = \hat{S} \hat{\Theta}(\lambda) \]
has the solution
\[ \hat{\Theta}(\lambda) = \hat{S} e^{\lambda \hat{S}} = \hat{S} e^{\lambda \hat{S}} \]
where $\hat{a}$ is an operator-valued integration constant. For $\hat{a} = \hat{1}$ we get $\hat{a}(\lambda) = e^{\lambda \hat{a}}$.

Be careful with handling exponentials of operators, though:

$$e^{\lambda \hat{a} \hat{b}} = e^{(\lambda + \beta) \hat{a}}$$

remains true, since $[\hat{a}, \hat{b}] = 0$.

but

$$e^{\lambda \hat{a} \hat{b}} \neq e^{\lambda \hat{a} + \beta \hat{b}}$$

unless $[\hat{a}, \hat{b}] = 0$!

Similarly

$$e^{\lambda \hat{a} \hat{b}} e^{\lambda \hat{a}} \neq e^{\lambda \hat{a}}$$

unless $[\hat{a}, \hat{b}] = 0$.

Chain rule for differentiation:

$$\frac{d}{d\lambda} e^{\lambda \hat{a} \hat{b}} e^{\lambda \hat{a}} = (\hat{a} e^{\lambda \hat{b}}) e^{\lambda \hat{a}} + e^{\lambda \hat{b}} (e^{\lambda \hat{a}} \hat{a})$$

$$= e^{\lambda \hat{a} \hat{b}} (\hat{a} + \hat{b}) e^{\lambda \hat{a}}$$

$$+ \hat{a} e^{\lambda \hat{a}} e^{\lambda \hat{b}} (\hat{a} + \hat{b})$$

$$= (\hat{a} + \hat{b}) e^{\lambda \hat{b}} e^{\lambda \hat{a}}.$$  

Differentiation with respect to operators:

If $\hat{F}(\hat{a}, \hat{b}, \ldots)$ is an operator-valued function of operators $\hat{a}, \hat{b}, \ldots$, we define the partial derivative of $\hat{F}$ with respect to $\hat{a}$ by

$$\frac{\partial \hat{F}}{\partial \hat{a}} = \lim_{\epsilon \to 0} \frac{\hat{F}(\hat{a} + \epsilon \hat{1}, \hat{b}, \ldots) - \hat{F}(\hat{a}, \hat{b}, \ldots)}{\epsilon}.$$
Using standard methods of calculus, it follows that

\[
\frac{\partial}{\partial \lambda} (F(\lambda) + G(\lambda)) = \frac{\partial F}{\partial \lambda} + \frac{\partial G}{\partial \lambda}
\]

\[
\frac{\partial}{\partial \lambda} (F \cdot G) = \frac{\partial F}{\partial \lambda} \cdot G + F \frac{\partial G}{\partial \lambda} \quad \text{(order of factors!!)}
\]

\[
\frac{d}{d\lambda} \lambda^n = n \lambda^{n-1} \Rightarrow \frac{d}{d\lambda} e^\lambda = \frac{d}{d\lambda} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} = \cdots = e^\lambda
\]

If \([\hat{\lambda}, \hat{\lambda}] = 0\) and \(F(\lambda) = \sum_{n=0}^{\infty} a_n \lambda^n\), then \([\hat{\lambda}, F] = 0\)

**Homework:**

\[
e^\hat{\lambda} e^{-\hat{\lambda}} = \sum_{n=0}^{\infty} \frac{1}{n!} [\hat{\lambda}, \hat{\lambda}]_{(n)}
\]

where \([\hat{\lambda}, \hat{\lambda}]_{(0)} = \hat{\lambda}\), \([\hat{\lambda}, \hat{\lambda}]_{(1)} = [\hat{\lambda}, \hat{\lambda}]\),

and \([\hat{\lambda}, \hat{\lambda}]_{(n)} = [\hat{\lambda}, [\hat{\lambda}, \hat{\lambda}]_{(n-1)}]\)

If \([\hat{\lambda}, [\lambda, \hat{\lambda}]] = 0 = [\hat{\lambda}, [\lambda, \hat{\lambda}]]\) (e.g. \([\hat{\lambda}, \hat{\lambda}] = \mu \hat{\lambda} - \text{a common occurrence}\))

then

\[
e^\hat{\lambda} + \hat{\alpha} = e^\lambda e^\hat{\lambda} - \frac{1}{2} [\hat{\lambda}, \hat{\lambda}]
\]