I.9 Functions of operators

Consider a function $f(x)$ ($x \in \mathbb{R}$ 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 $\hat{\Omega}$ through the corresponding series

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

This makes sense if the series somehow converges.
To see what this means, consider

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

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

$$\Omega \leftrightarrow \begin{pmatrix} \omega_1 & & & \\ & \omega_2 & & \\ & & \ddots & \\ & & & \omega_n \end{pmatrix}$$

Since from $\hat{\Omega}|\omega_i\rangle = \omega_i|\omega_i\rangle$ it follows that $\Omega^m|\omega_i\rangle = \omega_i^m|\omega_i\rangle$, $\hat{\Omega}^m$ is represented by $\hat{\Omega}^m = \begin{pmatrix} \omega_1^m & & & \\ & \omega_2^m & & \\ & & \ddots & \\ & & & \omega_n^m \end{pmatrix}$ and $e^{\hat{\Omega}}$ by

$$e^{\hat{\Omega}} \leftrightarrow \begin{pmatrix} \sum_{m=0}^{\infty} \frac{\omega_1^m}{m!} & & & \\ & \sum_{m=0}^{\infty} \frac{\omega_2^m}{m!} & & \\ & & \ddots & \\ & & & \sum_{m=0}^{\infty} \frac{\omega_n^m}{m!} \end{pmatrix} = \begin{pmatrix} e^{\omega_1} & & & \\ & e^{\omega_2} & & \\ & & \ddots & \\ & & & e^{\omega_n} \end{pmatrix}$$

So $f(\Omega) = \sum_{n=0}^{\infty} a_n \hat{\Omega}^n$ converges <u>iff</u>

$$f(\omega_i) = \sum_{n=0}^{\infty} a_n \omega_i^n \quad \text{converges for all eigenvalues } \omega_i.$$

Derivatives of operator w.r.t. parameters

For an operator $\hat{\theta}(\lambda)$, $\dfrac{d\hat{\theta}(\lambda)}{d\lambda} := \lim\limits_{\Delta\lambda \to 0} \dfrac{\hat{\theta}(\lambda+\Delta\lambda) - \hat{\theta}(\lambda)}{\Delta\lambda}$ ($\lambda \in \mathbb{R}$ is a parameter)

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

Important example:

$$\hat{\theta}(\lambda) = e^{\lambda \hat{\Omega}} \quad \text{with } \hat{\Omega} = \hat{\Omega}^{+}$$

By going to the eigenbasis of $\hat{\Omega}$ (where it is diagonal), one shows

$$\frac{d\hat{\theta}(\lambda)}{d\lambda} = \hat{\Omega} e^{\lambda \hat{\Omega}} = e^{\lambda \hat{\Omega}} = \hat{\theta}(\lambda)\hat{\Omega} = \hat{\Omega}\hat{\theta}(\lambda)$$

If $\hat{\Omega}$ is not Hermitian, look at the power series:

$$\frac{d}{d\lambda} \sum_{n=0}^{\infty} \frac{\lambda^n \hat{\Omega}^n}{n!} = \sum_{n=1}^{\infty} \frac{n \lambda^{n-1} \hat{\Omega}^n}{n!} = \hat{\Omega} \sum_{n=1}^{\infty} \frac{\lambda^{n-1} \hat{\Omega}^{n-1}}{(n-1)!} = \hat{\Omega} e^{\lambda \hat{\Omega}}$$

So the same holds true whenever the power series converges.

Conversely, the solution of the differential equation

$$\frac{d\hat{\theta}}{d\lambda} = \hat{\Omega}\, \hat{\theta}(\lambda)$$

has the solution $\hat{\theta}(\lambda) = \hat{c}\, e^{\int_0^{\lambda} d\lambda' \hat{\Omega}} = \hat{c}\, e^{\lambda \hat{\Omega}}$

where $\hat{C}$ is an operator-value integration constant.

For $\hat{C} = \hat{I}$ we get $\hat{\Theta}(\lambda) = e^{\lambda\hat{\Omega}}$

Be careful with handling exponentials of operators, though:

$$e^{\alpha\hat{\Omega}} e^{\beta\hat{\Omega}} = e^{(\alpha+\beta)\hat{\Omega}} \quad \text{remains true, since } [\hat{\Omega},\hat{\Omega}]=0$$

but $$e^{\alpha\hat{\Lambda}} e^{\beta\hat{\Omega}} \neq e^{\alpha\hat{\Lambda}+\beta\hat{\Omega}} \quad \text{unless } [\hat{\Lambda},\hat{\Omega}]=0 \ !$$

Similarly

$$e^{\alpha\hat{\Omega}} e^{\beta\hat{\Lambda}} e^{-\alpha\hat{\Omega}} \neq e^{\beta\hat{\Lambda}} \quad \text{unless } [\hat{\Lambda},\hat{\Omega}]=0.$$

Chain rule for differentiation:

$$\begin{aligned}\frac{d}{d\lambda} e^{\lambda\Omega} e^{\lambda\hat{\Theta}} &= (\Omega e^{\lambda\Omega}) e^{\lambda\hat{\Theta}} + e^{\lambda\hat{\Omega}}(e^{\lambda\hat{\Theta}}\hat{\Theta}) \\ &= e^{\lambda\hat{\Omega}}(\hat{\Omega}+\hat{\Theta}) e^{\lambda\hat{\Theta}} \\ &\neq e^{\lambda\hat{\Omega}} e^{\lambda\hat{\Theta}}(\hat{\Omega}+\hat{\Theta}) \\ &\neq (\hat{\Omega}+\hat{\Theta}) e^{\lambda\hat{\Omega}} e^{\lambda\hat{\Theta}} \quad !\end{aligned}$$

Differentiation with respect to operators:

If $\hat{F}(\hat{\Omega}_1, \hat{\Omega}_2, \dots)$ is an operator-valued function of operators $\hat{\Omega}_1, \hat{\Omega}_2, \dots$, we define the partial derivative of $\hat{F}$ with respect to $\hat{\Omega}_1$ by

$$\frac{\partial \hat{F}}{\partial \hat{\Omega}_1} = \lim_{\varepsilon \to 0} \frac{\hat{F}(\hat{\Omega}_1 + \varepsilon\hat{I}, \hat{\Omega}_2, \dots) - \hat{F}(\hat{\Omega}_1, \hat{\Omega}_2, \dots)}{\varepsilon}$$

Using standard methods of calculus, it follows that

$$\frac{\partial}{\partial\hat{\Lambda}}\left(\hat{F}(\hat{\Lambda})+\hat{G}(\hat{\Lambda})\right)=\frac{\partial\hat{F}}{\partial\hat{\Lambda}}+\frac{\partial\hat{G}}{\partial\hat{\Lambda}}$$

$$\frac{\partial}{\partial\hat{\Lambda}}\left(\hat{F}\,\hat{G}\right)=\frac{\partial\hat{F}}{\partial\hat{\Lambda}}\hat{G}+\hat{F}\frac{\partial\hat{G}}{\partial\hat{\Lambda}} \qquad \text{(order of factors!!)}$$

$$\frac{d}{d\hat{\Lambda}}\hat{\Lambda}^n=n\,\hat{\Lambda}^{n-1} \quad\Rightarrow\quad \frac{d}{d\hat{\Lambda}}e^{\hat{\Lambda}}=\frac{d}{d\hat{\Lambda}}\sum_{n=0}^{\infty}\frac{\hat{\Lambda}^n}{n!}=\dots=e^{\hat{\Lambda}}$$

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

Homework: $\boxed{e^{\hat{\Lambda}}\,\hat{\Omega}\,e^{-\hat{\Lambda}}=\sum_{n=0}^{\infty}\frac{1}{n!}[\hat{\Lambda},\hat{\Omega}]_{(n)}}$

where $[\hat{\Lambda},\hat{\Omega}]_{(0)}:=\hat{\Omega}$, $[\hat{\Lambda},\hat{\Omega}]_{(1)}=[\hat{\Lambda},\hat{\Omega}]$,

and $[\hat{\Lambda},\hat{\Omega}]_{(n)}=\left[\hat{\Lambda},[\hat{\Lambda},\hat{\Omega}]_{(n-1)}\right]$

If $[\hat{\Lambda},[\hat{\Lambda},\hat{\Omega}]]=0=[\hat{\Omega},[\hat{\Lambda},\hat{\Omega}]]$ (e.g. $[\hat{\Omega},\hat{\Lambda}]=\mu\hbar$ — a common occurrence)

then $\boxed{e^{\hat{\Lambda}+\hat{\Omega}}=e^{\hat{\Lambda}}\,e^{\hat{\Omega}}\,e^{-\frac{1}{2}[\hat{\Lambda},\hat{\Omega}]}}$