FUNCTIONS OF HERMITIAN OPERATORS

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.9.1 - 1.9.3.

One of the most common ways to define a function of an operator is to consider the case where the function can be expressed as a power series. That is, given an operator Ω, a function $f(\Omega)$ can be defined as

$$f(\Omega)=\sum_{n=0}^{\infty}a_n\Omega^n \tag{1}$$

where the coefficients a_n are, in general, complex scalars. This definition can still be difficult to deal with if Ω is not diagonalizable since, in that case, powers of Ω have no simple form, so it can be hard to tell if the series converges.

We can avoid this problem by restricting ourselves to hermitian operators, since such operators are always diagonalizable according to the spectral theorem and all eigenvalues of hermitian operators are real. Then powers of Ω are easy to calculate, since if the ith diagonal element of Ω is ω_i, the ith diagonal element of Ω^n is ω_i^n. The problem of finding $f(\Omega)$ is then reduced to examining whether the series converges for each diagonal element.

Example 1. Suppose we have the simplest such power series

$$f(\Omega)=\sum_{n=0}^{\infty}\Omega^n \tag{2}$$

If we look at this series in the eigenbasis (the basis of orthonormal eigenvectors that diagonalizes Ω), then we have

$$f(\Omega)=\left[\begin{array}{cccc}\sum_{n=0}^{\infty}\omega_1^n\\ & \sum_{n=0}^{\infty}\omega_2^n\\ & & \ddots\\ & & & \sum_{n=0}^{\infty}\omega_m^n\end{array}\right] \tag{3}$$

Ω here is an $m\times m$ matrix with eigenvalues ω_i, $i=1,\ldots,m$ (it's possible that some of the eigenvalues could be equal, if Ω is degenerate, but that doesn't affect the argument).

It's known that the geometric series

$$f(x)=\sum_{n=0}^{\infty}x^{n}=\frac{1}{1-x} \tag{4}$$

converges as shown, provided that $|x|<1$. Thus we see that $f(\Omega)$ converges provided all its eigenvalues satisfy $|\omega_i|<1$. The function is then

$$f(\Omega)=\begin{bmatrix}\frac{1}{1-\omega_1} & & & \\ & \frac{1}{1-\omega_2} & & \\ & & \ddots & \\ & & & \frac{1}{1-\omega_m}\end{bmatrix} \tag{5}$$

To see what operator it converges to, we consider the function

$$g(\Omega)=(I-\Omega)^{-1} \tag{6}$$

Still working in the eigenbasis where Ω is diagonal, the matrix $I-\Omega$ is also diagonal with diagonal elements $1-\omega_i$. The inverse of a diagonal matrix is another diagonal matrix with diagonal elements equal to the reciprocal of the elements in the original matrix, so $(I-\Omega)^{-1}$ has diagonal elements $\frac{1}{1-\omega_i}$ so from 5 we see that

$$f(\Omega)=\sum_{n=0}^{\infty}\Omega^{n}=(I-\Omega)^{-1} \tag{7}$$

provided all the eigenvalues of Ω satisfy $|\omega_i|<1$.

Example 2. If H is a hermitian operator, then e^{iH} is unitary. To see this, we again work in the eigenbasis of H. By expressing e^{iH} as a power series and using the same argument as in the previous example, we see that

$$U=e^{iH}=\begin{bmatrix}e^{i\omega_1} & & & \\ & e^{i\omega_2} & & \\ & & \ddots & \\ & & & e^{i\omega_m}\end{bmatrix} \tag{8}$$

The adjoint of e^{iH} is found by looking at the power series:

$$U^{\dagger}=\left(e^{iH}\right)^{\dagger}=\left[\sum_{n=0}^{\infty}\frac{(iH)^{n}}{n!}\right]^{\dagger} \tag{9}$$

$$=\sum_{n=0}^{\infty}\frac{\left(-iH^{\dagger}\right)^{n}}{n!} \tag{10}$$

$$=\sum_{n=0}^{\infty}\frac{(-iH)^{n}}{n!} \tag{11}$$

$$=e^{-iH} \tag{12}$$

where in the third line we used the hermitian property $H^{\dagger}=H$. Therefore

$$\left(e^{iH}\right)^{\dagger}=e^{-iH}=\begin{bmatrix} e^{-i\omega_1} & & & \\ & e^{-i\omega_2} & & \\ & & \ddots & \\ & & & e^{-i\omega_m}\end{bmatrix} \tag{13}$$

$$U^{\dagger}U=\left(e^{iH}\right)^{\dagger}e^{iH}=\begin{bmatrix} e^{-i\omega_1} & & & \\ & e^{-i\omega_2} & & \\ & & \ddots & \\ & & & e^{-i\omega_m}\end{bmatrix}\begin{bmatrix} e^{i\omega_1} & & & \\ & e^{i\omega_2} & & \\ & & \ddots & \\ & & & e^{i\omega_m}\end{bmatrix} \tag{14}$$

$$=I \tag{15}$$

Thus $\left(e^{iH}\right)^{\dagger}=\left(e^{iH}\right)^{-1}$ and e^{iH} is unitary.

From 8 we can find the determinant of e^{iH}:

$$\det U=\det e^{iH}=\exp\left[i\sum_{i=1}^{m}\omega_i\right]=\exp\left(i\operatorname{Tr}H\right) \tag{16}$$

since the trace of a hermitian matrix is the sum of its eigenvalues.

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