FUNCTIONS OF HERMITIAN OPERATORS

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A linear operator is defined in such a way that sums and products of operators have a meaning. That is, for operators A and B operating on a vector v, we have

$$\begin{aligned}(A+B)v &= Av+Bv \\ (AB)v &= A(Bv)\end{aligned} \tag{1}$$

Since these are the only ways we have of combining linear operators, how can we define a function $f(A)$ of a linear operator?

The most common ways to define such a function 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

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

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.

There are a couple of facts about functions of hermitian operators that are useful in quantum mechanics.

Theorem 1. *If H is a hermitian operator, then e^{iH} is unitary.*

Proof. To see this, we work in the eigenbasis of H, so that the matrix representation of H is diagonal. By expressing e^{iH} as a power series, we see that a function of H is a diagonal matrix with elements that are functions of the diagonal elements of H:

$$U = e^{iH} = \begin{bmatrix} e^{i\omega_1} & & & \\ & e^{i\omega_2} & & \\ & & \ddots & \\ & & & e^{i\omega_m} \end{bmatrix} \tag{3}$$

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

$$\begin{aligned} U^\dagger = \left(e^{iH}\right)^\dagger &= \left[\sum_{n=0}^{\infty} \frac{(iH)^n}{n!}\right]^\dagger & (4)\\ &= \sum_{n=0}^{\infty} \frac{\left(-iH^\dagger\right)^n}{n!} & (5)\\ &= \sum_{n=0}^{\infty} \frac{(-iH)^n}{n!} & (6)\\ &= e^{-iH} & (7) \end{aligned}$$

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

$$\left(e^{iH}\right)^\dagger = e^{-iH} = \begin{bmatrix} e^{-i\omega_1} & & & \\ & e^{-i\omega_2} & & \\ & & \ddots & \\ & & & e^{-i\omega_m} \end{bmatrix} \tag{8}$$

$$U^\dagger U = \left(e^{iH}\right)^\dagger e^{iH} = \begin{bmatrix} e^{-i\omega_1} & & & \\ & e^{-i\omega_2} & & \\ & & \ddots & \\ & & & e^{-i\omega_m} \end{bmatrix} \begin{bmatrix} e^{i\omega_1} & & & \\ & e^{i\omega_2} & & \\ & & \ddots & \\ & & & e^{i\omega_m} \end{bmatrix} \tag{9}$$

$$= I \tag{10}$$

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

From 3 we can find the determinant of e^{iH}:

$$\det U = \det e^{iH} = \exp\left[i\sum_{i=1}^{m} \omega_i\right] = \exp\left(i \mathrm{Tr} H\right) \tag{11}$$

since the trace of a hermitian matrix is the sum of its eigenvalues. To see this, suppose we have a hermitian matrix H that is not diagonal. We can diagonalize it in the usual way, by finding the matrix A whose columns are the eigenvectors of H. Then we have for the diagonal matrix H_D:

$$H_D = A^{-1} H A \tag{12}$$

Using the cyclic property of the trace, we have

$$\begin{aligned} \mathrm{Tr} H_D &= \mathrm{Tr}\left(A^{-1} H A\right) && (13)\\ &= \mathrm{Tr}\left(A A^{-1} H\right) && (14)\\ &= \mathrm{Tr} H && (15) \end{aligned}$$

Since the trace is the sum of the diagonal elements, and for a diagonal matrix, the diagonal elements are the eigenvalues, we see that the trace of a hermitian matrix is always the sum of its eigenvalues.

References

(1) Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press, Chapter 1.