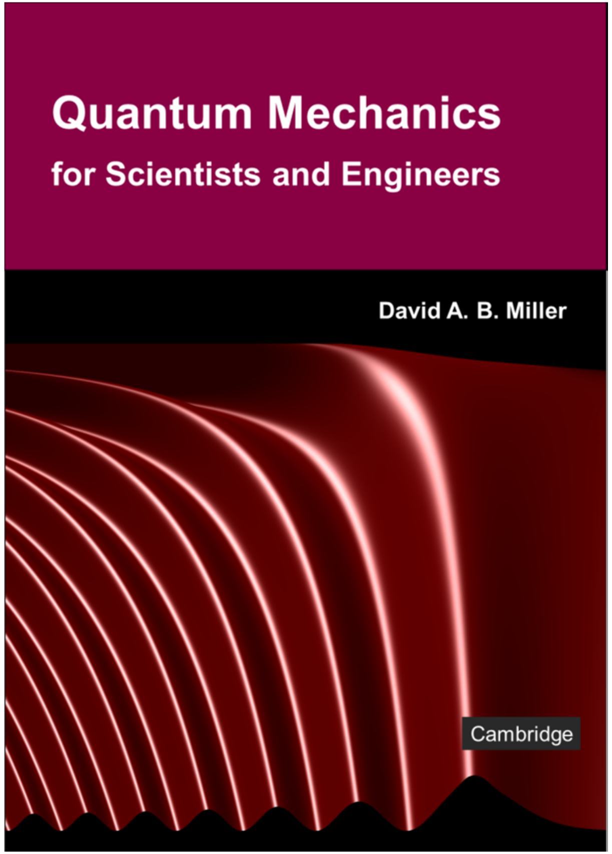
6.2 Unitary and Hermitian operators

Slides: Video 6.2.3 Hermitian operators

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.11



Unitary and Hermitian operators

Hermitian operators

Quantum mechanics for scientists and engineers

David Miller

Hermitian operators

A Hermitian operator is equal to its own Hermitian adjoint

$$\boxed{\hat{M}^{\dagger} = \hat{M}}$$

Equivalently it is self-adjoint

Hermitian operators

In matrix terms, with

$$\hat{M} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & \cdots \\ M_{21} & M_{22} & M_{23} & \cdots \\ M_{31} & M_{32} & M_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

then $\hat{M}^{\dagger} = \begin{bmatrix} M_{11}^{*} & M_{21}^{*} & M_{31}^{*} & \cdots \\ M_{12}^{*} & M_{22}^{*} & M_{31}^{*} & \cdots \\ M_{13}^{*} & M_{23}^{*} & M_{33}^{*} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$

so the Hermiticity implies $M_{ij} = M_{ji}^{*}$ for all i and j

so, also

the diagonal elements of a Hermitian operator must be real

Hermitian operators

To understand Hermiticity in the most general sense

consider

$$\langle g|\hat{M}|f\rangle$$

for arbitrary $|f\rangle$ and $|g\rangle$ and some operator $\hat{M}$

We examine

$$\left(\langle g|\hat{M}|f\rangle\right)^{\dagger}$$

Since this is just a number

a "1 x 1" matrix

it is also true that $\left(\langle g|\hat{M}|f\rangle\right)^{\dagger} \equiv \left(\langle g|\hat{M}|f\rangle\right)^{*}$

Hermitian operators

We can also analyze $\left(\langle g|\hat{M}|f\rangle\right)^{\dagger}$ using the rule $\left(\hat{A}\hat{B}\right)^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$ for Hermitian adjoints of products

So $\left(\langle g|\hat{M}|f\rangle\right)^{*} \equiv \left(\langle g|\hat{M}|f\rangle\right)^{\dagger} = \left(\hat{M}|f\rangle\right)^{\dagger}\left(\langle g|\right)^{\dagger} = \left(|f\rangle\right)^{\dagger}\hat{M}^{\dagger}\left(\langle g|\right)^{\dagger}$

$$= \langle f|\hat{M}^{\dagger}|g\rangle$$

Hence, if $\hat{M}$ is Hermitian, with therefore $\hat{M}^{\dagger} = \hat{M}$

then

$$\boxed{\left(\langle g|\hat{M}|f\rangle\right)^{*} = \langle f|\hat{M}|g\rangle}$$

even if $|f\rangle$ and $|g\rangle$ are not orthogonal

This is the most general statement of Hermiticity

Hermitian operators

In integral form, for functions $f(x)$ and $g(x)$

the statement $\left(\langle g|\hat{M}|f\rangle\right)^* = \langle f|\hat{M}|g\rangle$ can be written

$$\int g^*(x)\hat{M}f(x)\,dx = \left[\int f^*(x)\hat{M}g(x)\,dx\right]^*$$

We can rewrite the right hand side using $(ab)^* = a^*b^*$

$$\int g^*(x)\hat{M}f(x)\,dx = \int f(x)\left\{\hat{M}g(x)\right\}^*\,dx$$

and a simple rearrangement leads to

$$\int g^*(x)\hat{M}f(x)\,dx = \int \left\{\hat{M}g(x)\right\}^* f(x)\,dx$$

which is a common statement of Hermiticity in integral form

Bra-ket and integral notations

Note that in the bra-ket notation

the operator can also be considered to operate to the left

$\langle g | \hat{A}$ is just as meaningful a statement as $\hat{A} | f \rangle$

and we can group the bra-ket multiplications as we wish

$$\langle g | \hat{A} | f \rangle \equiv \left(\langle g | \hat{A} \right) | f \rangle \equiv \langle g | \left(\hat{A} | f \rangle \right)$$

Conventional operators in the notation used in integration

such as a differential operator, d/dx

do not have any meaning operating "to the left"

so Hermiticity in this notation is the less elegant form

$$\int g^*(x) \hat{M} f(x) dx = \int \left\{ \hat{M} g(x) \right\}^* f(x) dx$$

Reality of eigenvalues

Suppose $|\psi_n\rangle$ is a normalized eigenvector of the Hermitian operator $\hat{M}$ with eigenvalue μ_n

Then, by definition

$$\hat{M}|\psi_n\rangle = \mu_n|\psi_n\rangle$$

Therefore

$$\langle\psi_n|\hat{M}|\psi_n\rangle = \mu_n\langle\psi_n|\psi_n\rangle = \mu_n$$

But from the Hermiticity of $\hat{M}$ we know

$$\langle\psi_n|\hat{M}|\psi_n\rangle = \left(\langle\psi_n|\hat{M}|\psi_n\rangle\right)^* = \mu_n^*$$

and hence μ_n must be real

Orthogonality of eigenfunctions for different eigenvalues

Trivially $\quad 0 = \langle \psi_m | \hat{M} | \psi_n \rangle - \langle \psi_m | \hat{M} | \psi_n \rangle$

By associativity $\quad 0 = \left(\langle \psi_m | \hat{M} \right) | \psi_n \rangle - \langle \psi_m | \left(\hat{M} | \psi_n \rangle \right)$

Using $\left(\hat{A}\hat{B} \right)^\dagger = \hat{B}^\dagger \hat{A}^\dagger$ $\quad 0 = \left(\hat{M}^\dagger | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \left(\hat{M} | \psi_n \rangle \right)$

Using Hermiticity $\hat{M} = \hat{M}^\dagger$ $\quad 0 = \left(\hat{M} | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \left(\hat{M} | \psi_n \rangle \right)$

Using $\hat{M} | \psi_n \rangle = \mu_n | \psi_n \rangle$ $\quad 0 = \left(\mu_m | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \mu_n | \psi_n \rangle$

μ_m and μ_n are real numbers $\quad 0 = \mu_m \left(| \psi_m \rangle \right)^\dagger | \psi_n \rangle - \mu_n \langle \psi_m || \psi_n \rangle$

Rearranging $\quad 0 = \left(\mu_m - \mu_n \right) \langle \psi_m | \psi_n \rangle$

But μ_m and μ_n are different, so $0 = \langle \psi_m | \psi_n \rangle$ i.e., orthogonality

Degeneracy

It is quite possible
- and common in symmetric problems
  - to have more than one eigenfunction
    - associated with a given eigenvalue

This situation is known as degeneracy
- It is provable that
  - the number of such degenerate solutions
    - for a given finite eigenvalue
      - is itself finite