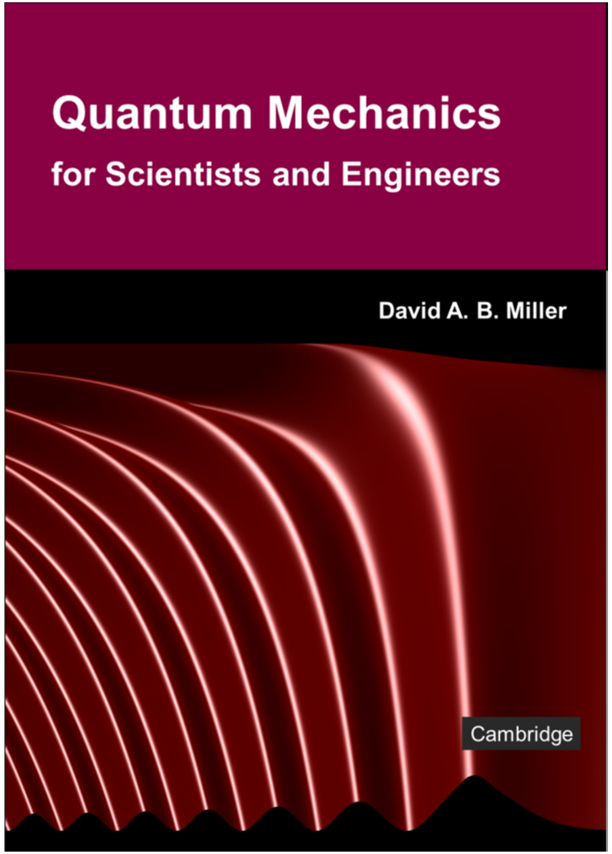
6.2 Unitary and Hermitian operators

Slides: Video 6.2.1 Using unitary operators

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.10 (starting from "Changing the representation of vectors")



Unitary and Hermitian operators

Using unitary operators

Quantum mechanics for scientists and engineers

David Miller

Unitary operators to change representations of vectors

Suppose that we have a vector (function) $|f_{old}\rangle$

that is represented

when expressed as an expansion on

the functions $|\psi_n\rangle$

as the mathematical column vector $|f_{old}\rangle = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$

These numbers c_1, c_2, c_3, ...

are the projections of $|f_{old}\rangle$

on the orthogonal coordinate axes

in the vector space

labeled with $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$ ...

Unitary operators to change representations of vectors

Suppose we want to represent this vector on a new set of orthogonal axes

- which we will label $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ ...

Changing the axes

- which is equivalent to changing the basis set of functions
  - does not change the vector we are representing
    - but it does change
      - the column of numbers used to represent the vector

Unitary operators to change representations of vectors

For example, suppose the original vector $|f_{old}\rangle$

was actually the first basis vector in the old basis $|\psi_1\rangle$

Then in this new representation

the elements in the column of numbers

would be the projections of this vector

on the various new coordinate axes

each of which is simply $\langle\phi_m|\psi_1\rangle$

So under this coordinate transformation

or change of basis

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix} \Rightarrow \begin{bmatrix} \langle\phi_1|\psi_1\rangle \\ \langle\phi_2|\psi_1\rangle \\ \langle\phi_3|\psi_1\rangle \\ \vdots \end{bmatrix}$$

Unitary operators to change representations of vectors

Writing similar transformations for each basis vector $|\psi_n\rangle$

we get the correct transformation

if we define a matrix

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

where $u_{ij} = \langle \phi_i | \psi_j \rangle$

and we define our new column of numbers $|f_{new}\rangle$

$$|f_{new}\rangle = \hat{U}|f_{old}\rangle$$

Unitary operators to change representations of vectors

Note incidentally that here

$|f_{old}\rangle$ and $|f_{new}\rangle$ are the same vector in the vector space

Only the representation

the coordinate axes

and, consequently

the column of numbers

that have changed

not the vector itself

Unitary operators to change representations of vectors

Now we can prove that $\hat{U}$ is unitary

Writing the matrix multiplication in its sum form

$$\left(\hat{U}^{\dagger}\hat{U}\right)_{ij} = \sum_m u_{mi}^* u_{mj} = \sum_m \langle \phi_m | \psi_i \rangle^* \langle \phi_m | \psi_j \rangle = \sum_m \langle \psi_i | \phi_m \rangle \langle \phi_m | \psi_j \rangle$$

$$= \langle \psi_i | \left(\sum_m |\phi_m\rangle\langle\phi_m| \right) | \psi_j \rangle = \langle \psi_i | \hat{I} | \psi_j \rangle = \langle \psi_i | \psi_j \rangle = \delta_{ij}$$

so $\hat{U}^{\dagger}\hat{U} = \hat{I}$

hence $\hat{U}$ is unitary

since its Hermitian transpose is therefore its inverse

Unitary operators to change representations of vectors

Hence any change in basis

can be implemented with a unitary operator

We can also say that

any such change in representation to a new orthonormal basis

is a unitary transform

Note also, incidentally, that

$$\hat{U}\hat{U}^{\dagger} = \left(\hat{U}^{\dagger}\hat{U}\right)^{\dagger} = \hat{I}^{\dagger} = \hat{I}$$

so the mathematical order of this multiplication makes no difference

Unitary operators to change representations of operators

Consider a number such as $\langle g|\hat{A}|f\rangle$

where vectors $|f\rangle$ and $|g\rangle$ and operator $\hat{A}$ are arbitrary

This result should not depend on the coordinate system

so the result in an "old" coordinate system $\langle g_{old}|\hat{A}_{old}|f_{old}\rangle$

should be the same in a "new" coordinate system

that is, we should have $\langle g_{new}|\hat{A}_{new}|f_{new}\rangle = \langle g_{old}|\hat{A}_{old}|f_{old}\rangle$

Note the subscripts "new" and "old" refer to representations

not the vectors (or operators) themselves

which are not changed by change of representation

Only the numbers that represent them are changed

Unitary operators to change representations of operators

With unitary $\hat{U}$ operator to go from "old" to "new" systems

we can write $\langle g_{new} | \hat{A}_{new} | f_{new} \rangle = \left(| g_{new} \rangle \right)^{\dagger} \hat{A}_{new} | f_{new} \rangle$

$$= \left(\hat{U} | g_{old} \rangle \right)^{\dagger} \hat{A}_{new} \left(\hat{U} | f_{old} \rangle \right) = \langle g_{old} | \hat{U}^{\dagger} \hat{A}_{new} \hat{U} | f_{old} \rangle$$

Since we believe also that $\langle g_{new} | \hat{A}_{new} | f_{new} \rangle = \langle g_{old} | \hat{A}_{old} | f_{old} \rangle$

then we identify $\hat{A}_{old} = \hat{U}^{\dagger} \hat{A}_{new} \hat{U}$

or since $\hat{U} \hat{A}_{old} \hat{U}^{\dagger} = \left(\hat{U} \hat{U}^{\dagger} \right) \hat{A}_{new} \left(\hat{U} \hat{U}^{\dagger} \right) = \hat{A}_{new}$

then $\boxed{\hat{A}_{new} = \hat{U} \hat{A}_{old} \hat{U}^{\dagger}}$

Unitary operators that change the state vector

For example, if the quantum mechanical state $|\psi\rangle$

is expanded on the basis $|\psi_n\rangle$ to give $|\psi\rangle = \sum_n a_n |\psi_n\rangle$

then $\sum_n |a_n|^2 = 1$

and if the particle is to be conserved

then this sum is retained as the quantum mechanical system evolves in time

But this is just the square of the vector length

Hence a unitary operator, which conserves length

describes changes that conserve the particle