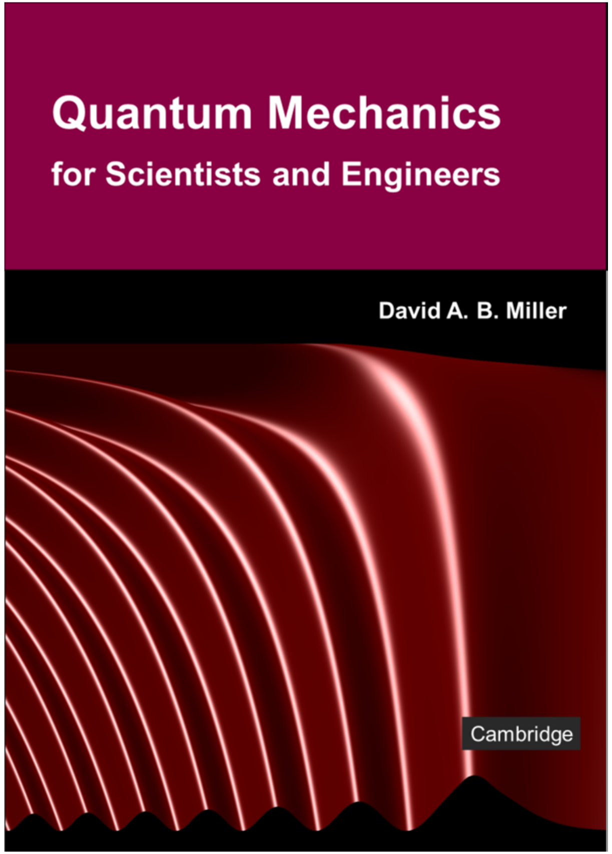
5.3 Vector spaces, operators and matrices

Slides: Video 5.3.5 Linear operators and their algebra

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 4.4 – 4.5



Vector spaces, operators and matrices

Linear operators and their algebra

Quantum mechanics for scientists and engineers

David Miller

Consequences of linear operator algebra

Because of the mathematical equivalence of matrices and linear operators

the algebra for such operators

is identical to that of matrices

In particular

operators do not in general commute

$\hat{A}\hat{B}|f\rangle$ is not in general equal to $\hat{B}\hat{A}|f\rangle$

for any arbitrary $|f\rangle$

Whether or not operators commute

is very important in quantum mechanics

Generalization to expansion coefficients

We discussed operators

for the case of functions of position (e.g., x)

but we can also use expansion coefficients on basis sets

We expanded $f(x) = \sum_n c_n \psi_n(x)$ and $g(x) = \sum_n d_n \psi_n(x)$

We could have followed a similar argument

requiring each expansion coefficient d_i

depends linearly on all the expansion coefficients c_n

Generalization to expansion coefficients

By similar arguments

we would deduce the most general linear relation

between the vectors of expansion coefficients

could be represented as a matrix

$$\begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$$

The bra-ket statement of the relation between f, g, and $\hat{A}$ remains unchanged as $|g\rangle = \hat{A}|f\rangle$

Evaluating the matrix elements of an operator

Now we will find out how we can write some operator

as a matrix

That is, we will deduce how to calculate all the elements of the matrix

if we know the operator

Suppose we choose our function $f(x)$

to be the *j*th basis function $\psi_j(x)$

so $f(x) = \psi_j(x)$ or equivalently $|f\rangle = |\psi_j\rangle$

Evaluating the matrix elements of an operator

Then, in the expansion $f(x) = \sum_n c_n \psi_n(x)$

we are choosing $c_j = 1$

with all the other c's being 0

Now we operate on this $|f\rangle$ with $\hat{A}$

in $|g\rangle = \hat{A}|f\rangle$

to get $|g\rangle$

Suppose specifically

we want to know the resulting coefficient d_i

in the expansion $g(x) = \sum_n d_n \psi_n(x)$

Evaluating the matrix elements of an operator

From the matrix form of $|g\rangle = \hat{A}|f\rangle$

$$\begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$$

with our choice $c_j = 1$ and all other c's 0 then

we would have

$$d_i = A_{ij}$$

Evaluating the matrix elements of an operator

For example, for $j = 2$

that is, $c_2 = 1$ and all other c's 0 then

$$\begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{12} \\ A_{22} \\ A_{32} \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

so in this example

$$d_3 = A_{32}$$

Evaluating the matrix elements of an operator

But, from the expansions for $|f\rangle$ and $|g\rangle$

for the specific case of $|f\rangle = |\psi_j\rangle$

$$|g\rangle = \sum_n d_n |\psi_n\rangle = \hat{A}|f\rangle = \hat{A}|\psi_j\rangle$$

To extract d_i from this expression

we multiply by $\langle\psi_i|$ on both sides to obtain

$$d_i = \langle\psi_i|\hat{A}|\psi_j\rangle$$

But we already concluded for this case that $d_i = A_{ij}$

So $$A_{ij} = \langle\psi_i|\hat{A}|\psi_j\rangle$$

Evaluating the matrix elements of an operator

But our choices of i and j here were arbitrary

So quite generally

when writing an operator $\hat{A}$ as a matrix

when using a basis set $|\psi_n\rangle$

the matrix elements of that operator are

$$\boxed{A_{ij} = \langle \psi_i | \hat{A} | \psi_j \rangle}$$

We can now turn any linear operator into a matrix

For example, for a simple one-dimensional spatial case

$$A_{ij} = \int \psi_i^*(x) \hat{A} \psi_j(x) dx$$

Visualization of a matrix element

Operator $\hat{A}$

acting on the unit vector $|\psi_j\rangle$

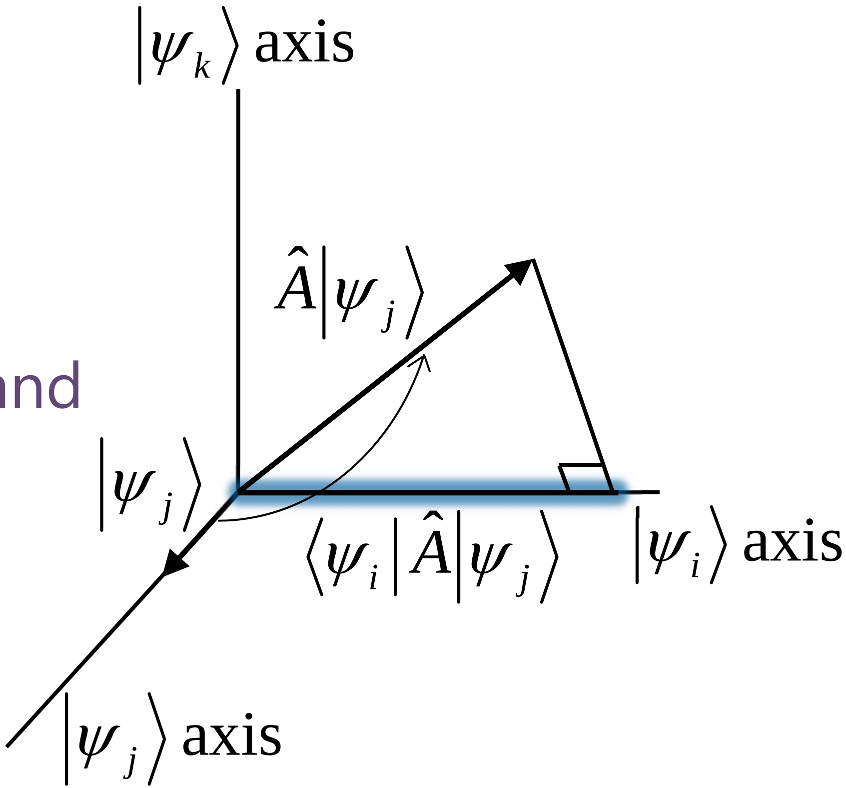
generates the vector $\hat{A}|\psi_j\rangle$

with generally a new length and direction

The matrix element $\langle\psi_i|\hat{A}|\psi_j\rangle$

is the projection of $\hat{A}|\psi_j\rangle$

onto the $|\psi_i\rangle$ axis



Evaluating the matrix elements

We can write the matrix for the operator $\hat{A}$

$$\hat{A} \equiv \begin{bmatrix} \langle \psi_1 | \hat{A} | \psi_1 \rangle & \langle \psi_1 | \hat{A} | \psi_2 \rangle & \langle \psi_1 | \hat{A} | \psi_3 \rangle & \cdots \\ \langle \psi_2 | \hat{A} | \psi_1 \rangle & \langle \psi_2 | \hat{A} | \psi_2 \rangle & \langle \psi_2 | \hat{A} | \psi_3 \rangle & \cdots \\ \langle \psi_3 | \hat{A} | \psi_1 \rangle & \langle \psi_3 | \hat{A} | \psi_2 \rangle & \langle \psi_3 | \hat{A} | \psi_3 \rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

We have now deduced how to set up

a function as a vector and

a linear operator as a matrix

which can operate on the vectors