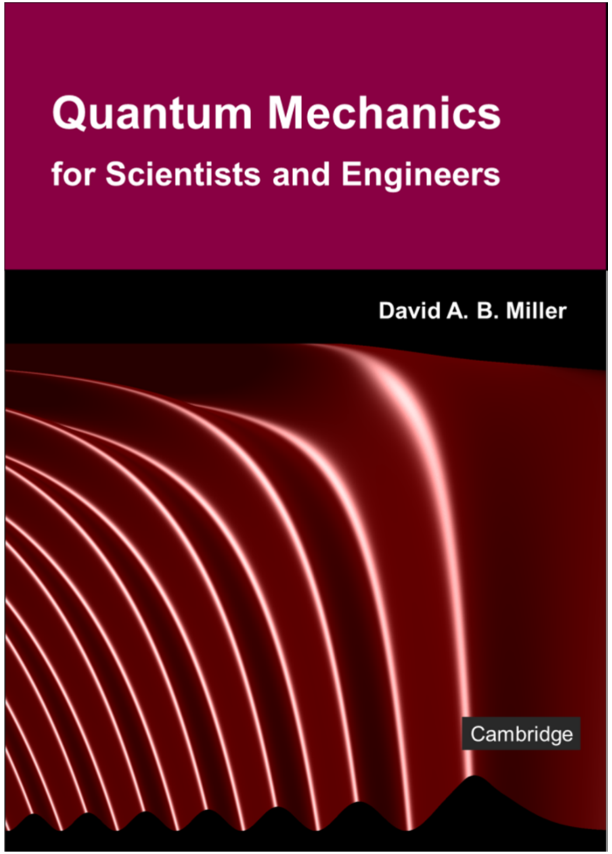
5.3 Vector spaces, operators and matrices

Slides: Video 5.3.3 Operators

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 4.3 – 4.4



Vector spaces, operators and matrices

Operators

Quantum mechanics for scientists and engineers

David Miller

Operators

A function turns one number

- the argument
  - into another
    - the result

An operator turns one function into another

- In the vector space representation of a function
  - an operator turns one vector into another

Operators

Suppose that we are constructing the new function $g(y)$

from the function $f(x)$

by acting on $f(x)$

with the operator $\hat{A}$

The variables x and y might be the same kind of variable

as in the case where the operator corresponds to differentiation of the function

$$g(x) = \left(\frac{d}{dx}\right) f(x)$$

Operators

The variables x and y might be quite different

as in the case of a Fourier transform operation where

x might represent time and

y might represent frequency

$$g(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-iyx)\, dx$$

A standard notation for writing any such operation on a function is

$$g(y) = \hat{A} f(x)$$

This should be read as $\hat{A}$ operating on $f(x)$

Operators

For $\hat{A}$ to be the most general operation possible

it should be possible for the value of $g(y)$

for example, at some particular value of $y = y_1$

to depend on the values of $f(x)$

for all values of the argument x

This is the case, for example, in the Fourier transform operation

$$g(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-iyx)\, dx$$

Linear operators

We are interested here solely in linear operators

- They are the only ones we will use in quantum mechanics
  - because of the fundamental linearity of quantum mechanics

A linear operator has the following characteristics

$$\hat{A}\left[f(x)+h(x)\right]=\hat{A}f(x)+\hat{A}h(x)$$

$$\hat{A}\left[cf(x)\right]=c\hat{A}f(x)$$

for any complex number c

Consequences of linearity for operators

Let us consider the most general way we could have the function $g(y)$

at some specific value y_1 of its argument

that is, $g(y_1)$

be related to the values of $f(x)$

for possibly all values of x

and still retain the linearity properties for this relation

Consequences of linearity for operators

Think of the function $f(x)$

as being represented by a list of values

$f(x_1)$, $f(x_2)$, $f(x_3)$, … ,

just as we did when considering $f(x)$ as a vector

We can take the values of x to be as closely spaced as we want

We believe that this representation can give us as accurate a representation of $f(x)$

for any calculation we need to perform

Consequences of linearity for operators

Then we propose that

for a linear operation

the value of $g(y_1)$

might be related to the values of $f(x)$

by a relation of the form

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$$

where the a_{ij} are complex constants

Consequences of linearity for operators

This form $g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$

shows the linearity behavior we want

If we replaced $f(x)$ by $f(x) + h(x)$

then we would have

$$g(y_1) = a_{11}\left[f(x_1) + h(x_1)\right] + a_{12}\left[f(x_2) + h(x_2)\right] + a_{13}\left[f(x_3) + h(x_3)\right] + \ldots$$

$$= a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$$

$$+ a_{11} h(x_1) + a_{12} h(x_2) + a_{13} h(x_3) + \ldots$$

as required for a linear operator relation from

$$\hat{A}\left[f(x) + h(x)\right] = \hat{A} f(x) + \hat{A} h(x)$$

Consequences of linearity for operators

And, in this form $g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$

if we replaced $f(x)$ by $cf(x)$

then we would have

$$g(y_1) = a_{11} cf(x_1) + a_{12} cf(x_2) + a_{13} cf(x_3) + \ldots$$

$$= c\left[a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots\right]$$

as required for a linear operator relation from

$$\hat{A}\left[cf(x)\right] = c\hat{A}f(x)$$

Consequences of linearity for operators

Now consider whether this form

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$$

is as general as it could be and still be a linear relation

We can see this by trying to add other powers and "cross terms" of $f(x)$

Any more complicated relation of $g(y_1)$ to $f(x)$

could presumably be written as a power series in $f(x)$

possibly involving $f(x)$

for different values of x

that is, "cross terms"

Consequences of linearity for operators

If we were to add higher powers of $f(x)$

such as $\left[f(x)\right]^2$

or cross terms such as $f(x_1)f(x_2)$

into the series $g(y_1)=a_{11}f(x_1)+a_{12}f(x_2)+a_{13}f(x_3)+\ldots$

it would no longer have the required linear behavior of

$$\hat{A}\left[f(x)+h(x)\right]=\hat{A}f(x)+\hat{A}h(x)$$

We also cannot add a constant term to this series

That would violate the second linearity condition

$$\hat{A}\left[cf(x)\right]=c\hat{A}f(x)$$

The additive constant would not be multiplied by c

Generality of the proposed linear operation

Hence we conclude

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$$

is the most general form possible

for the relation between $g(y_1)$

and $f(x)$

if this relation is to correspond to a linear operator

Construction of the entire operator

To construct the entire function $g(y)$

we should construct series like

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$$

for each value of y

If we write $f(x)$ and $g(y)$ as vectors

then we can write all these series at once

$$\begin{bmatrix} g(y_1) \\ g(y_2) \\ g(y_3) \\ \vdots \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \end{bmatrix}$$

Construction of the entire operator

We see that $\begin{bmatrix} g(y_1) \\ g(y_2) \\ g(y_3) \\ \vdots \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \end{bmatrix}$

can be written as $g(y) = \hat{A} f(x)$

where the operator $\hat{A}$ can be written as a matrix

$$\hat{A} \equiv \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Bra-ket notation and operators

Presuming functions can be represented as vectors

then linear operators can be represented by matrices

In bra-ket notation, we can write $g(y) = \hat{A} f(x)$ as

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

If we regard the ket as a vector

we now regard the (linear) operator $\hat{A}$

as a matrix