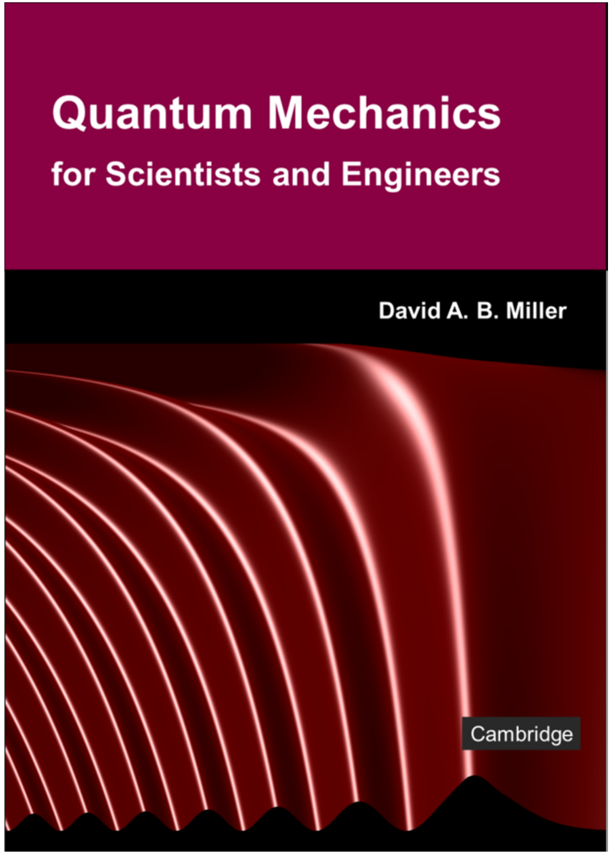
5.2 Functions and Dirac notation

Slides: Video 5.2.5 Using Dirac notation

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.1 (remainder of 4.1)



Functions and Dirac notation

Using Dirac notation

Quantum mechanics for scientists and engineers

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Bra-ket notation and expansions on basis sets

Suppose the function is not represented directly

as a set of values for each point in space

but is expanded in a complete orthonormal basis $\psi_n(x)$

$$f(x) = \sum_n c_n \psi_n(x)$$

We could also write the function as the "ket" $|f(x)\rangle \equiv \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$

(with possibly an infinite number of elements)

In this case, the "bra" version becomes

$$\langle f(x)| \equiv \begin{bmatrix} c_1^* & c_2^* & c_3^* & \cdots \end{bmatrix}$$

Bra-ket notation and expansions on basis sets

When we write the function in this different form

as a vector containing these expansion coefficients

we say we have changed its "representation"

The function $f(x)$ is still the same function

the vector $|f(x)\rangle$ is the same vector in our space

We have just changed the axes we use to represent the function

so the coordinates of the vector have changed

now they are the numbers c_1, c_2, c_3

Bra-ket notation and expansions on basis sets

Just as before, we could evaluate

$$\int \left| f(x) \right|^2 dx \equiv \int f^*(x) f(x) dx \equiv \int \left[\sum_n c_n^* \psi_n^*(x) \right] \left[\sum_m c_m \psi_m(x) \right] dx$$

$$\equiv \sum_{n,m} c_n^* c_m \int \psi_n^*(x) \psi_m(x) dx \equiv \sum_{n,m} c_n^* c_m \delta_{nm} \equiv \sum_n \left| c_n \right|^2$$

$$\equiv \begin{bmatrix} c_1^* & c_2^* & c_3^* & \cdots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix} \equiv \langle f(x) | f(x) \rangle$$

so the answer is the same no matter how we write it

Bra-ket notation and expansions on basis sets

Similarly, with

$$g(x) = \sum_n d_n \psi_n(x)$$

we have

$$\int g^*(x) f(x) dx \equiv \begin{bmatrix} d_1^* & d_2^* & d_3^* & \cdots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$$

$$\equiv \langle g(x) | f(x) \rangle$$

Bra-ket expressions

Note that the result of a bra-ket expression like

$$\left\langle f(x) \middle| f(x) \right\rangle \quad \text{or} \quad \left\langle g(x) \middle| f(x) \right\rangle$$

is simply a number (in general, complex)

which is easy to see if we think of this as a vector multiplication

Note that this number is not changed as we change the representation

just as the dot product of two vectors

is independent of the coordinate system

Expansion coefficients

Evaluating the c_n in $$f(x) = \sum_n c_n \psi_n(x)$$

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

is simple because the functions $\psi_n(x)$ are orthonormal

Since $\psi_n(x)$ is just a function

we can also write it as a ket $|\psi_n\rangle$

To evaluate the coefficient c_m

we premultiply by the bra $\langle\psi_m|$ to get

$$\langle\psi_m(x)|f(x)\rangle = \sum_n c_n \langle\psi_m(x)|\psi_n(x)\rangle = \sum_n c_n \delta_{mn} = c_m$$

Expansion coefficients

Using bra-ket notation

we can write $f(x)=\sum_n c_n \psi_n(x)$ as

$$\left|f(x)\right\rangle = \sum_n c_n \left|\psi_n(x)\right\rangle = \sum_n \left|\psi_n(x)\right\rangle c_n = \sum_n \left|\psi_n(x)\right\rangle \left\langle \psi_n(x) \middle| f(x)\right\rangle$$

Because c_n is just a number

it can be moved about in the product

Multiplication of vectors and numbers is commutative

Often in using the bra-ket notation

we may drop arguments like x

Then we can write $\left|f\right\rangle = \sum_n c_n \left|\psi_n\right\rangle = \sum_n \left|\psi_n\right\rangle c_n = \sum_n \left|\psi_n\right\rangle \left\langle \psi_n \middle| f\right\rangle$

State vectors

In quantum mechanics

- where the function f represents the state of the quantum mechanical system
  - such as the wavefunction
    - the set of numbers represented by the bra $\langle f|$ or ket $|f\rangle$ vector
      - represents the state of the system

Hence we refer to

- $|f\rangle$ as the "state vector" of the system
  - and $\langle f|$ as the (Hermitian) adjoint of the state vector

State vectors

In quantum mechanics

the bra or ket always represents either

the quantum mechanical state of the system

such as the spatial wavefunction $\psi(x)$

or some state the system could be in

such as one of the basis states $\psi_n(x)$

Convention for symbols in bra and ket vectors

The convention for what is inside the bra or ket is loose

usually one deduces from the context what is meant

For example

if it is obvious what basis we were working with

we might use $|n\rangle$ to represent the nth basis function (or basis "state")

rather than the notation $|\psi_n(x)\rangle$ or $|\psi_n\rangle$

The symbols inside the bra or ket should be enough to make it clear what state we are discussing

Otherwise there are essentially no rules for the notation

Convention for symbols in bra and ket vectors

For example, we could write

$$\left| \begin{array}{l} \text{The state where the electron has the lowest} \\ \text{possible energy in a harmonic oscillator with} \\ \text{potential energy } 0.375x^2 \end{array} \right\rangle$$

but since we likely already know we are discussing such a harmonic oscillator

it will save us time and space simply to write $|0\rangle$

with 0 representing the quantum number

Either would be correct mathematically