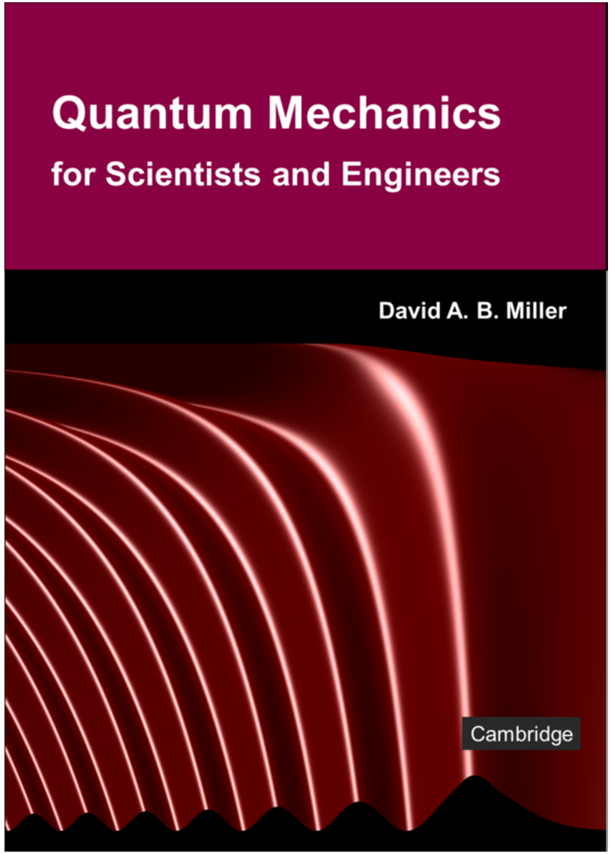
5.2 Functions and Dirac notation

Slides: Video 5.2.3 Dirac notation

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.1 (first part of “Dirac bra-ket notation”)



Functions and Dirac notation

Dirac notation

Quantum mechanics for scientists and engineers

David Miller

Dirac bra-ket notation

The first part of the Dirac "bra-ket" notation $|f(x)\rangle$

called a "ket"

refers to our column vector

For the case of our function $f(x)$

one way to define the "ket" is $|f(x)\rangle \equiv \begin{bmatrix} f(x_1)\sqrt{\delta x} \\ f(x_2)\sqrt{\delta x} \\ f(x_3)\sqrt{\delta x} \\ \vdots \end{bmatrix}$

or the limit of this as $\delta x \to 0$

We put $\sqrt{\delta x}$ into the vector for normalization

The function is still a vector list of numbers

Dirac bra-ket notation

We can similarly define the "bra" $\langle f(x)|$

to refer a row vector

$$\langle f(x)| \equiv \left[f^*(x_1)\sqrt{\delta x} \quad f^*(x_2)\sqrt{\delta x} \quad f^*(x_3)\sqrt{\delta x} \quad \cdots \right]$$

where we mean the limit of this as $\delta x \to 0$

Note that, in our row vector

we take the complex conjugate of all the values

Note that this "bra" refers to exactly the same function as the "ket"

These are different ways of writing the same function

Hermitian adjoint

The vector $\begin{bmatrix} a_1^* & a_2^* & a_3^* & \cdots \end{bmatrix}$

is called, variously

the Hermitian adjoint

the Hermitian transpose

the Hermitian conjugate

the adjoint

of the vector $\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}$

Hermitian adjoint

A common notation used to indicate the Hermitian adjoint

is to use the character "†" as a superscript

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}^\dagger = \begin{bmatrix} a_1^* & a_2^* & a_3^* & \cdots \end{bmatrix}$$

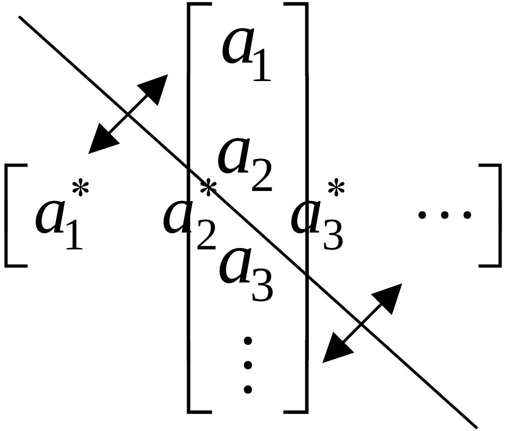
Hermitian adjoint

Forming the Hermitian adjoint is like

reflecting about a -45º line

then taking the complex conjugate of all the elements

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}^\dagger \Rightarrow$$



$$= \begin{bmatrix} a_1^* & a_2^* & a_3^* & \cdots \end{bmatrix}$$

Hermitian adjoint and bra-ket notation

The "bra" is the Hermitian adjoint of the "ket"

and *vice versa*

$$\left(|f\rangle\right)^\dagger = \langle f| \qquad \left(\langle f|\right)^\dagger = |f\rangle$$

The Hermitian adjoint of the Hermitian adjoint

brings us back to where we started

$$\left(\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}^\dagger\right)^\dagger = \begin{bmatrix} a_1^* & a_2^* & a_3^* & \cdots \end{bmatrix}^\dagger = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}$$

Bra-ket notation for functions

Considering $f(x)$ as a vector

and following our previous result

and adding bra-ket notation

$$\int |f(x)|^2 dx \equiv \begin{bmatrix} f^*(x_1)\sqrt{\delta x} & f^*(x_2)\sqrt{\delta x} & f^*(x_3)\sqrt{\delta x} & \cdots \end{bmatrix} \begin{bmatrix} f(x_1)\sqrt{\delta x} \\ f(x_2)\sqrt{\delta x} \\ f(x_3)\sqrt{\delta x} \\ \vdots \end{bmatrix}$$

$$\equiv \sum_n f^*(x_n)\sqrt{\delta x}\, f(x_n)\sqrt{\delta x}$$

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

where again the strict equality applies in the limit when $\delta x \to 0$

Bra-ket notation for functions

Note that the use of the bra-ket notation here

eliminates the need to write an integral or a sum

The sum is implicit in the vector multiplication

$$\int \left| f(x) \right|^2 dx \equiv \begin{bmatrix} f^*(x_1)\sqrt{\delta x} & f^*(x_2)\sqrt{\delta x} & f^*(x_3)\sqrt{\delta x} & \cdots \end{bmatrix} \begin{bmatrix} f(x_1)\sqrt{\delta x} \\ f(x_2)\sqrt{\delta x} \\ f(x_3)\sqrt{\delta x} \\ \vdots \end{bmatrix}$$

$$\equiv \sum_n f^*(x_n)\sqrt{\delta x}\, f(x_n)\sqrt{\delta x}$$

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

Bra-ket notation for functions

Note the shorthand for the vector product of the "bra" and "ket"

$$\langle g | \times | f \rangle \equiv \langle g | f \rangle$$

The middle vertical line is usually omitted

though it would not matter if it was still there

Bra-ket notation for functions

This notation is also useful for integrals of two different functions

$$\int g^*(x) f(x) dx \equiv \begin{bmatrix} g^*(x_1)\sqrt{\delta x} & g^*(x_2)\sqrt{\delta x} & g^*(x_3)\sqrt{\delta x} & \cdots \end{bmatrix} \begin{bmatrix} f(x_1)\sqrt{\delta x} \\ f(x_2)\sqrt{\delta x} \\ f(x_3)\sqrt{\delta x} \\ \vdots \end{bmatrix}$$

$$\equiv \sum_n g^*(x_n)\sqrt{\delta x}\, f(x_n)\sqrt{\delta x}$$

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

Inner product

In general this kind of "product" $\langle g|\times|f\rangle \equiv \langle g|f\rangle$

is called an inner product in linear algebra

The geometric vector dot product is an inner product

The bra-ket "product" $\langle g|f\rangle$ is an inner product

The "overlap integral" $\int g^*(x)\,f(x)\,dx$ is an inner product

Inner product

It is "inner" because

- it takes two vectors and turns them into a number
  - a "smaller" entity

In the Dirac notation $\langle g | f \rangle$

- the bra-ket gives an inner "feel" to this product
  - The special parentheses give a "closed" look