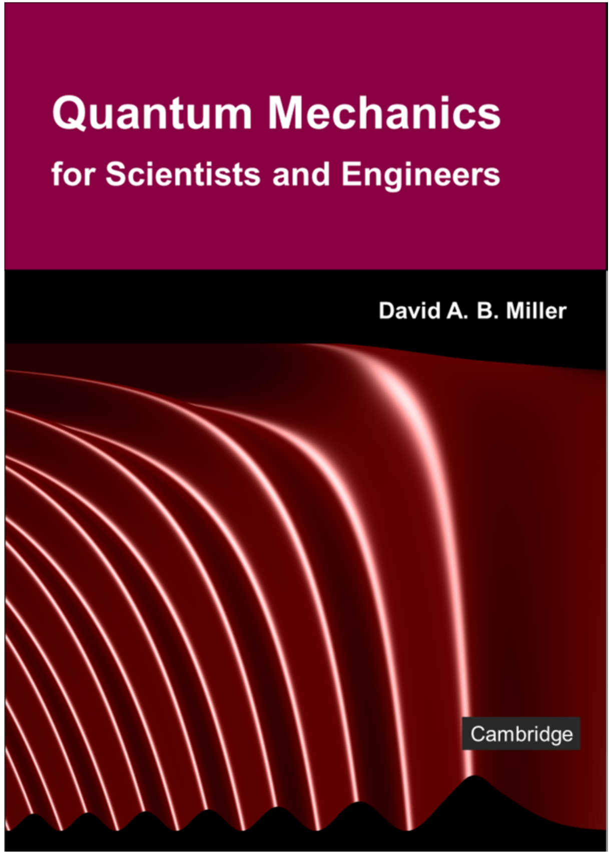
5.2 Functions and Dirac notation

Slides: Video 5.2.1 Introduction to functions and Dirac notation

Text reference: Quantum Mechanics for Scientists and Engineers

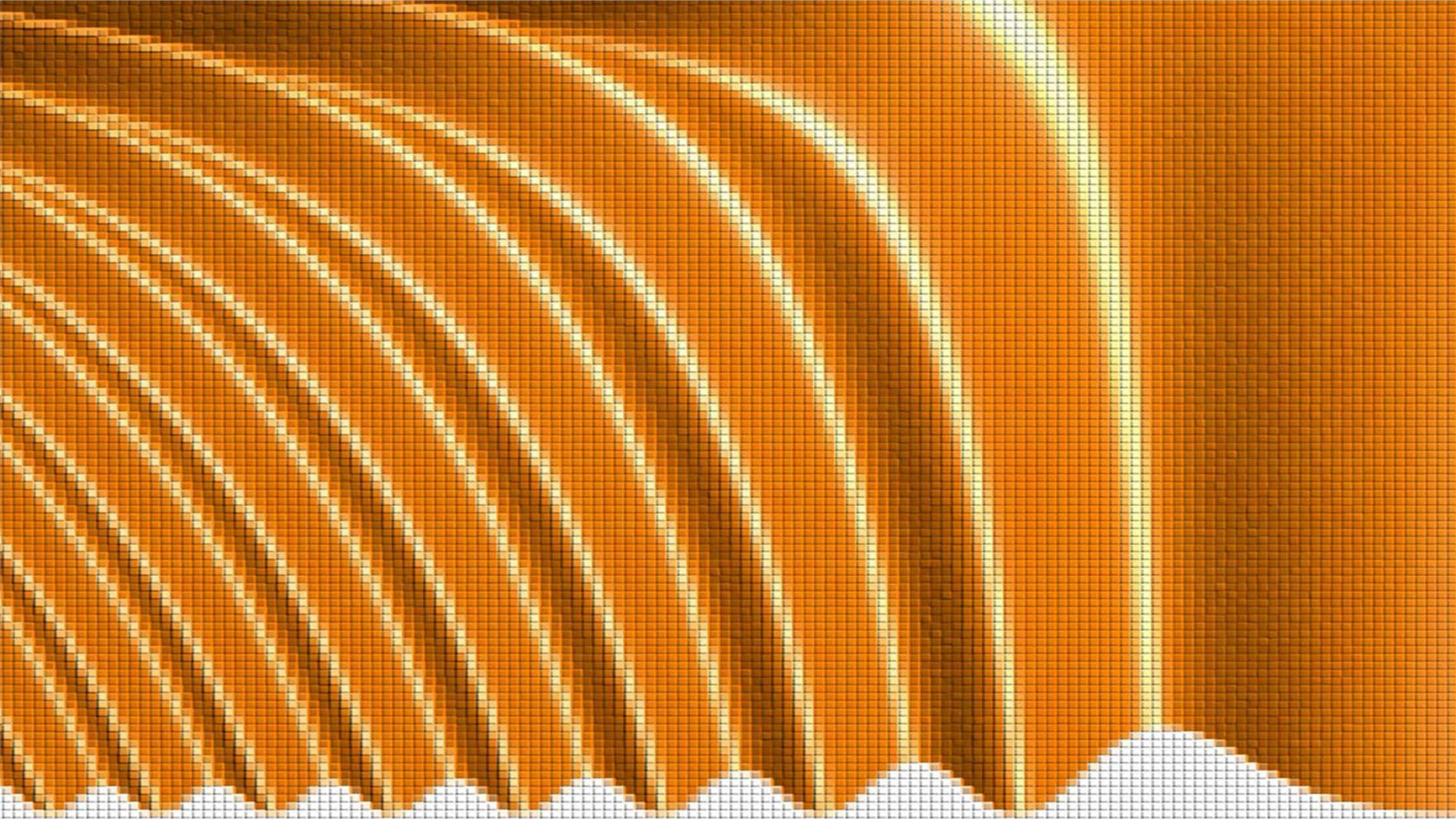
Chapter 4 introduction



Functions and Dirac notation

Quantum mechanics for scientists and engineers

David Miller

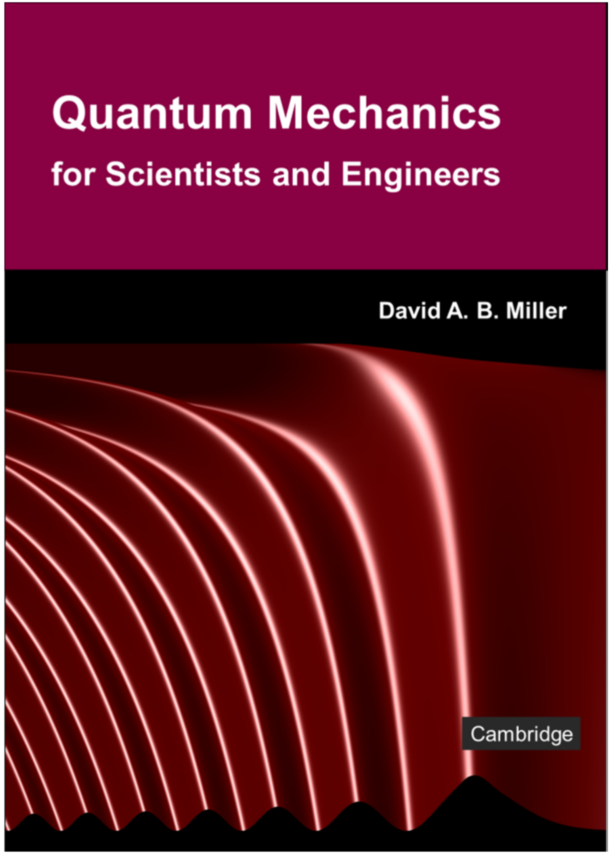


5.2 Functions and Dirac notation

Slides: Video 5.2.2 Functions as vectors

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.1 (up to "Dirac bra-ket notation")



Functions and Dirac notation

Functions as vectors

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Functions as vectors

One kind of list of arguments would be the list of all real numbers

- which we could list in order as

  - $x_1, x_2, x_3 \ldots$

  - and so on

This is an infinitely long list

- and the adjacent values in the list

  - are infinitesimally close together

    - but we will regard these infinities as details!

Functions as vectors

If we presume that we know this list of possible arguments of the function

we can write out the function as the corresponding list of values, and

we choose to write this list as a column vector

$$\begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \end{bmatrix}$$

Functions as vectors

For example

- we could specify the function at points spaced by some small amount δx
  - with $x_2 = x_1 + \delta x$, $x_3 = x_2 + \delta x$ and so on

We would do this

- for sufficiently many values of x and
  - over a sufficient range of x
    - to get a sufficiently useful representation for some calculation
      - such as an integral

Functions as vectors

The integral of $\left| f\left(x\right) \right|^2$

could then be written as

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

Provided we choose δx sufficiently small

and the corresponding vectors therefore sufficiently long

we can get an arbitrarily good approximation to the integral

Visualizing a function as a vector

Suppose the function $f(x)$ is approximated by its values at three points

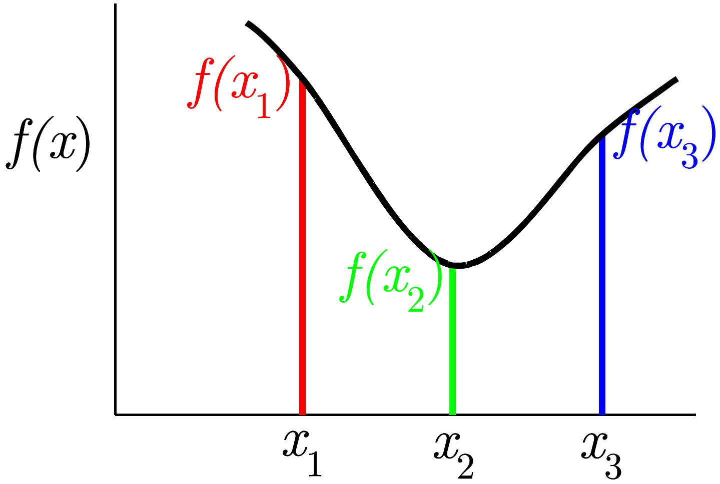
x_1, x_2, and x_3

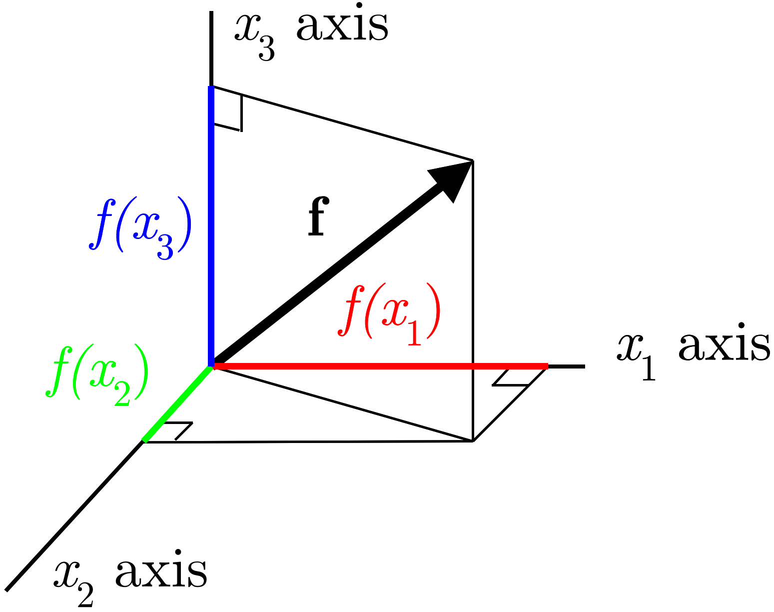
and is represented as a vector

$$\mathbf{f} \equiv \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{bmatrix}$$

then we can visualize the function as a vector in ordinary geometrical space

Visualizing a function as a vector



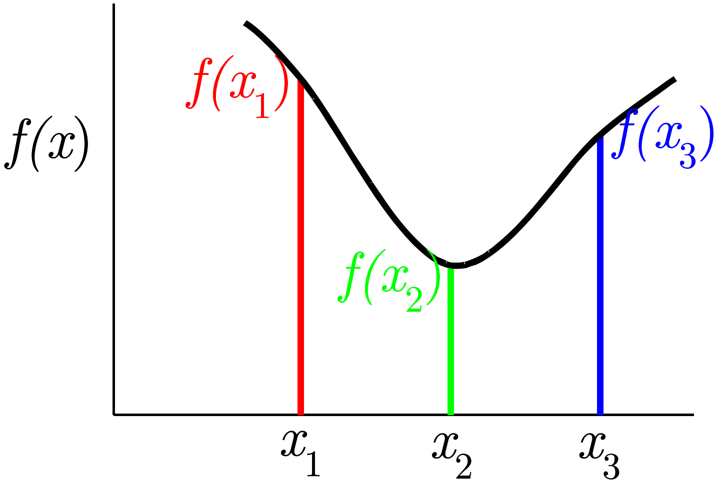


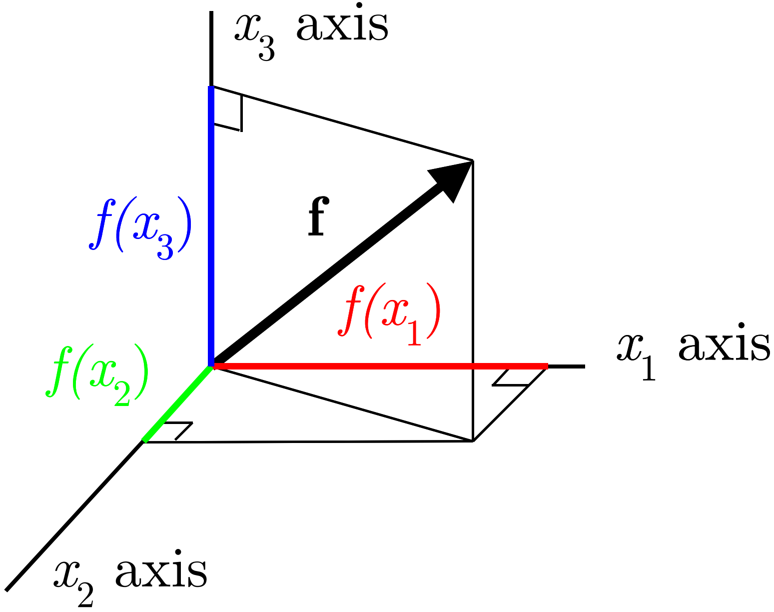
We could draw a vector

whose components along three axes

were the values of the function at these three points

Visualizing a function as a vector





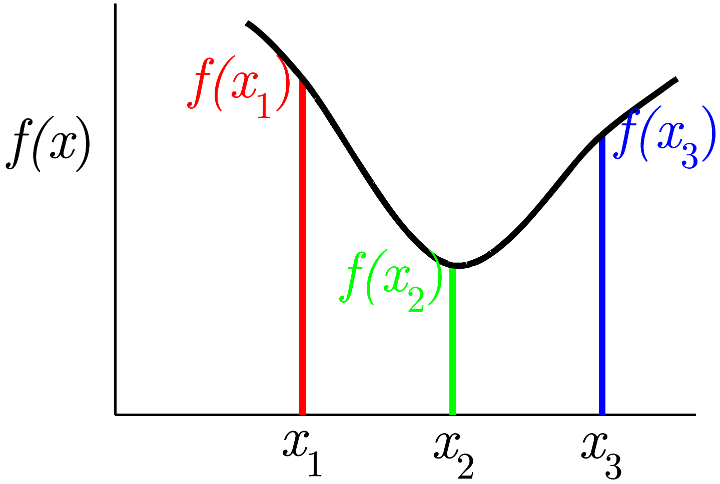
In quantum mechanics

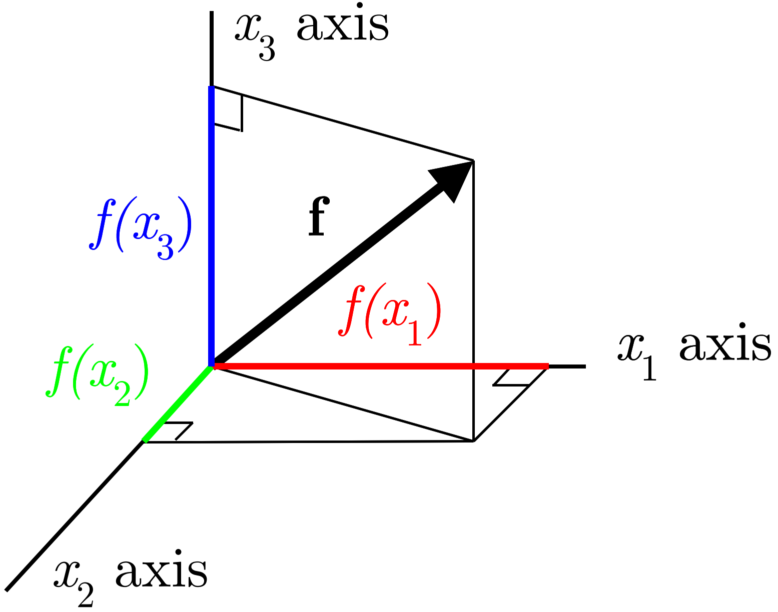
the functions are complex, not merely real

and there may be many elements in the vector

possibly an infinite number

Visualizing a function as a vector

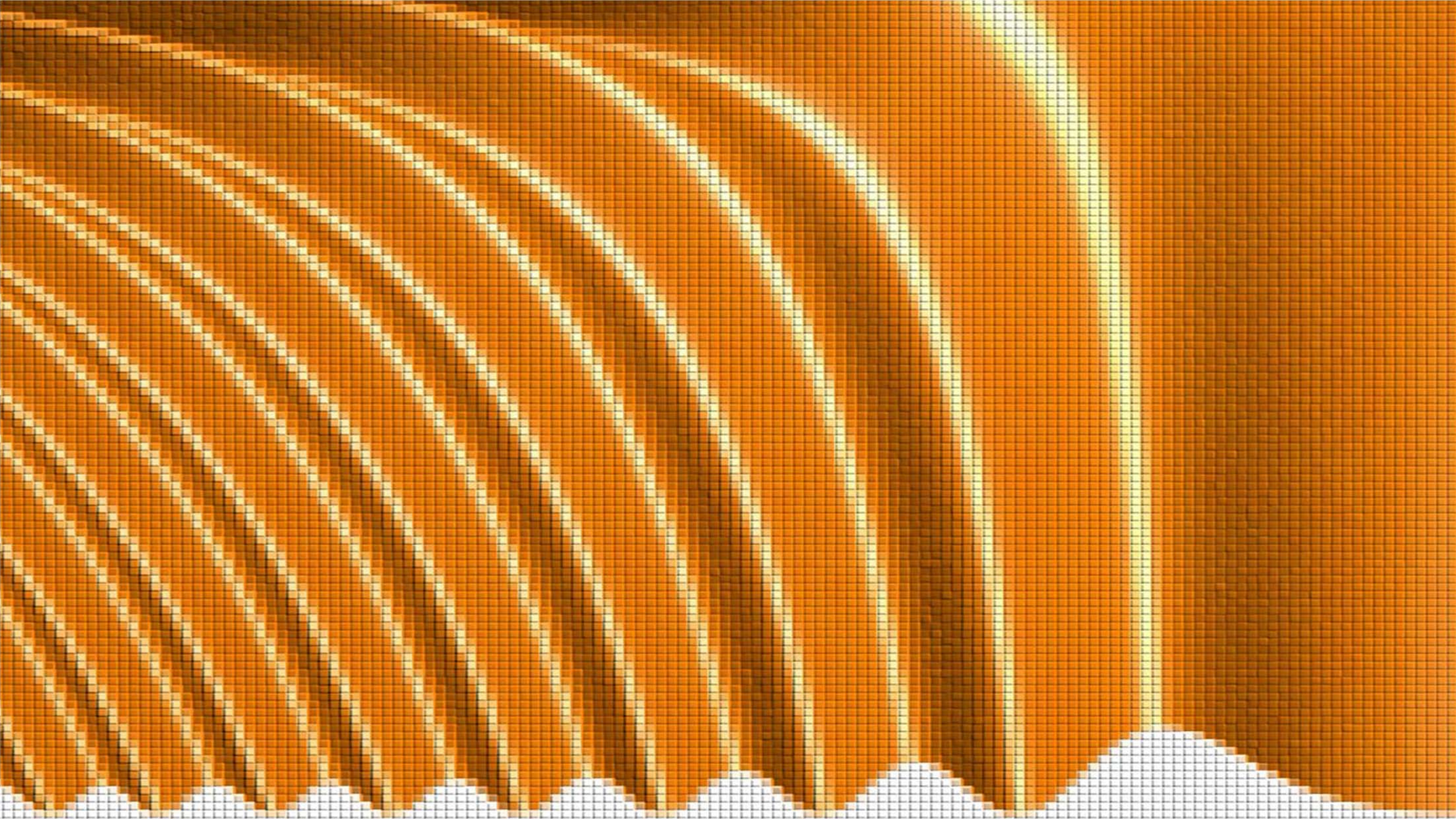




But we will still visualize the function

and, more generally, the quantum mechanical state

as a vector in a space

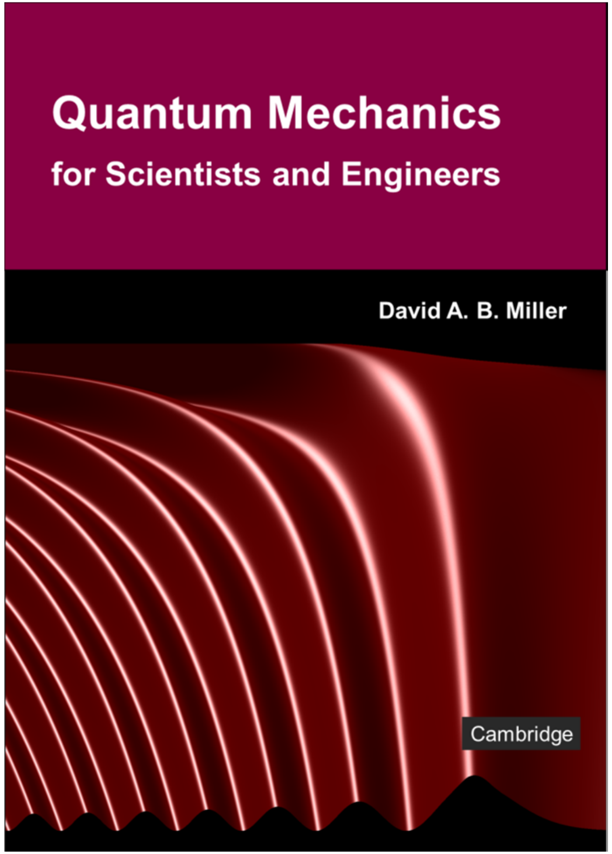


5.2 Functions and Dirac notation

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 $\left| f(x) \right\rangle$

called a "ket"

refers to our column vector

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

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

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 -45° line

then taking the complex conjugate of all the elements

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

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

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

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

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

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

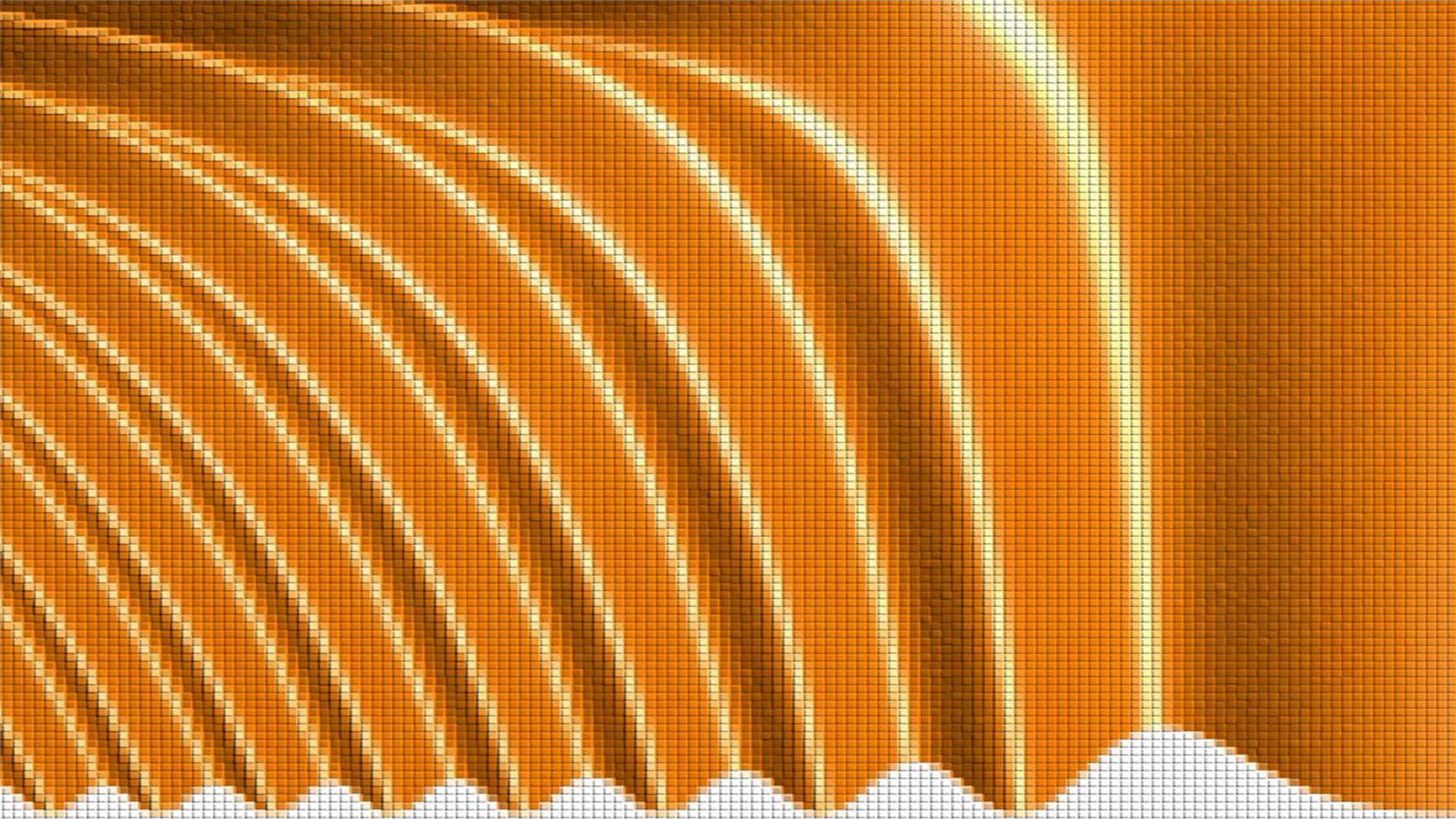
Inner product

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

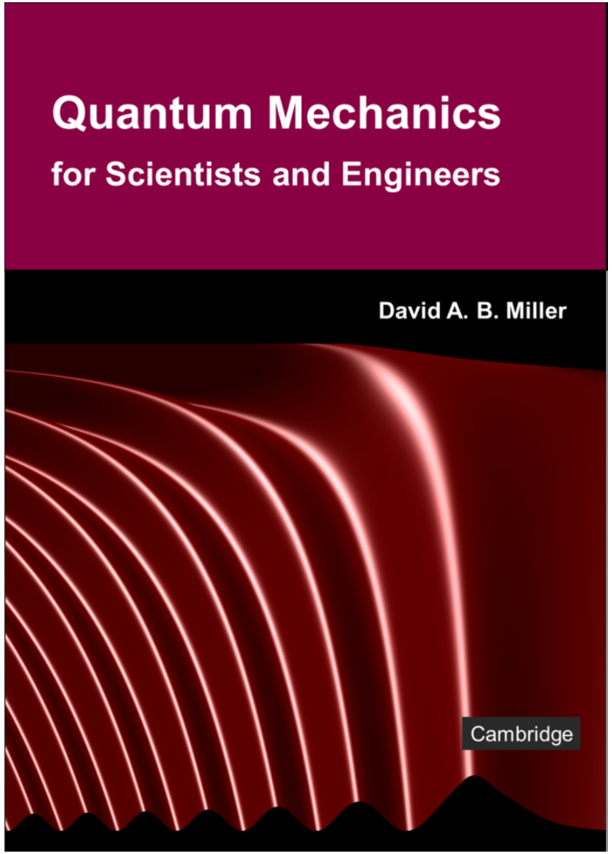


5.2 Functions and Dirac notation

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

David Miller

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" $\left| f(x) \right\rangle \equiv \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$

(with possibly an infinite number of elements)

In this case, the "bra" version becomes

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

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

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

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

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

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