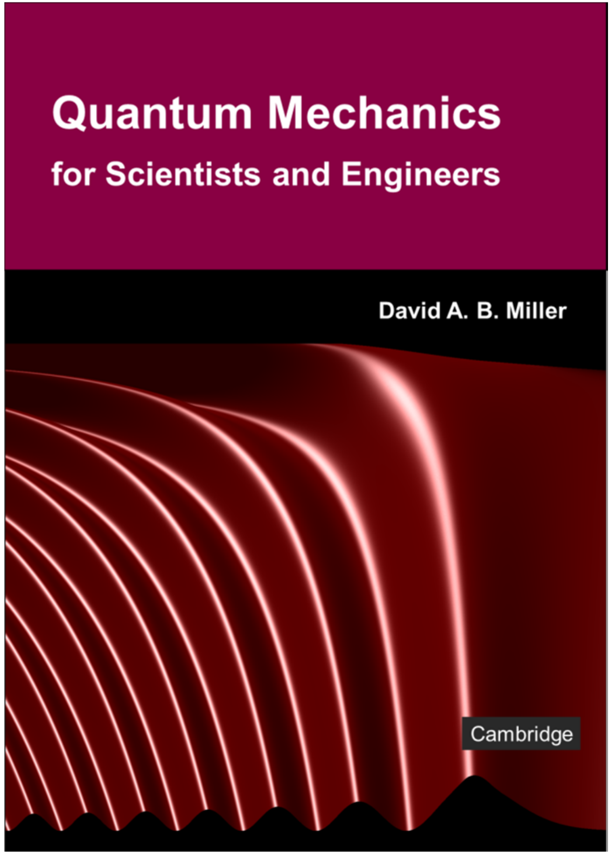
6.1 Types of linear operators

Slides: Video 6.1.1 Bilinear expansion of operators

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.6



Types of linear operators

Bilinear expansion of operators

Quantum mechanics for scientists and engineers

David Miller

Bilinear expansion of linear operators

We know that we can expand functions in a basis set

as in $f(x)=\sum_n c_n \psi_n(x)$ or $\left|f(x)\right\rangle=\sum_n c_n \left|\psi_n(x)\right\rangle$

What is the equivalent expansion for an operator?

We can deduce this from our matrix representation

Consider an arbitrary function *f*, written as the ket $\left|f\right\rangle$

from which we can calculate a function g

written as the ket $\left|g\right\rangle$

by acting with a specific operator $\hat{A}$

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

Bilinear expansion of linear operators

We expand g and f on the basis set ψ_i

$$\left|g\right\rangle = \sum_i d_i \left|\psi_i\right\rangle \qquad \left|f\right\rangle = \sum_j c_j \left|\psi_j\right\rangle$$

From our matrix representation of $\left|g\right\rangle = \hat{A}\left|f\right\rangle$

we know that $d_i = \sum_j A_{ij} c_j$

and, by definition of the expansion coefficient

we know that $c_j = \left\langle \psi_j \middle| f \right\rangle$

so $d_i = \sum_j A_{ij} \left\langle \psi_j \middle| f \right\rangle$

Bilinear expansion of linear operators

Substituting $d_i = \sum_j A_{ij} \langle \psi_j | f \rangle$ back into $|g\rangle = \sum_i d_i |\psi_i\rangle$ gives

$$|g\rangle = \sum_{i,j} A_{ij} \langle \psi_j | f \rangle |\psi_i\rangle$$

Remember that $\langle \psi_j | f \rangle \equiv c_j$ is simply a number

so we can move it within the multiplicative expression

Hence we have $|g\rangle = \sum_{i,j} A_{ij} |\psi_i\rangle \langle \psi_j | f \rangle = \left[\sum_{i,j} A_{ij} |\psi_i\rangle \langle \psi_j | \right] | f \rangle$

But $|g\rangle = \hat{A} | f \rangle$ and $|g\rangle$ and $| f \rangle$ are arbitrary, so

$$\hat{A} \equiv \sum_{i,j} A_{ij} |\psi_i\rangle \langle \psi_j |$$

Bilinear expansion of linear operators

This form

$$\hat{A} \equiv \sum_{i,j} A_{ij} |\psi_i\rangle\langle\psi_j|$$

is referred to as

a "bilinear expansion" of the operator $\hat{A}$

on the basis $|\psi_i\rangle$

and is analogous to the linear expansion of a vector on a basis

Any linear operator that operates within the space can be written this way

Bilinear expansion of linear operators

Though the Dirac notation is more general and elegant

for functions of a simple variable where

$$g(x) = \int \hat{A} f(x_1)\, dx_1$$

we can analogously write the bilinear expansion in the form

$$\hat{A} \equiv \sum_{i,j} A_{ij} \psi_i(x) \psi_j^*(x_1)$$

Outer product

An expression of the form

$$\hat{A} \equiv \sum_{i,j} A_{ij} \left|\psi_i\right\rangle\left\langle\psi_j\right|$$

contains an *outer* product of two vectors

An inner product expression of the form $\langle g | f \rangle$

results in a single, complex number

An outer product expression of the form $|g\rangle\langle f|$

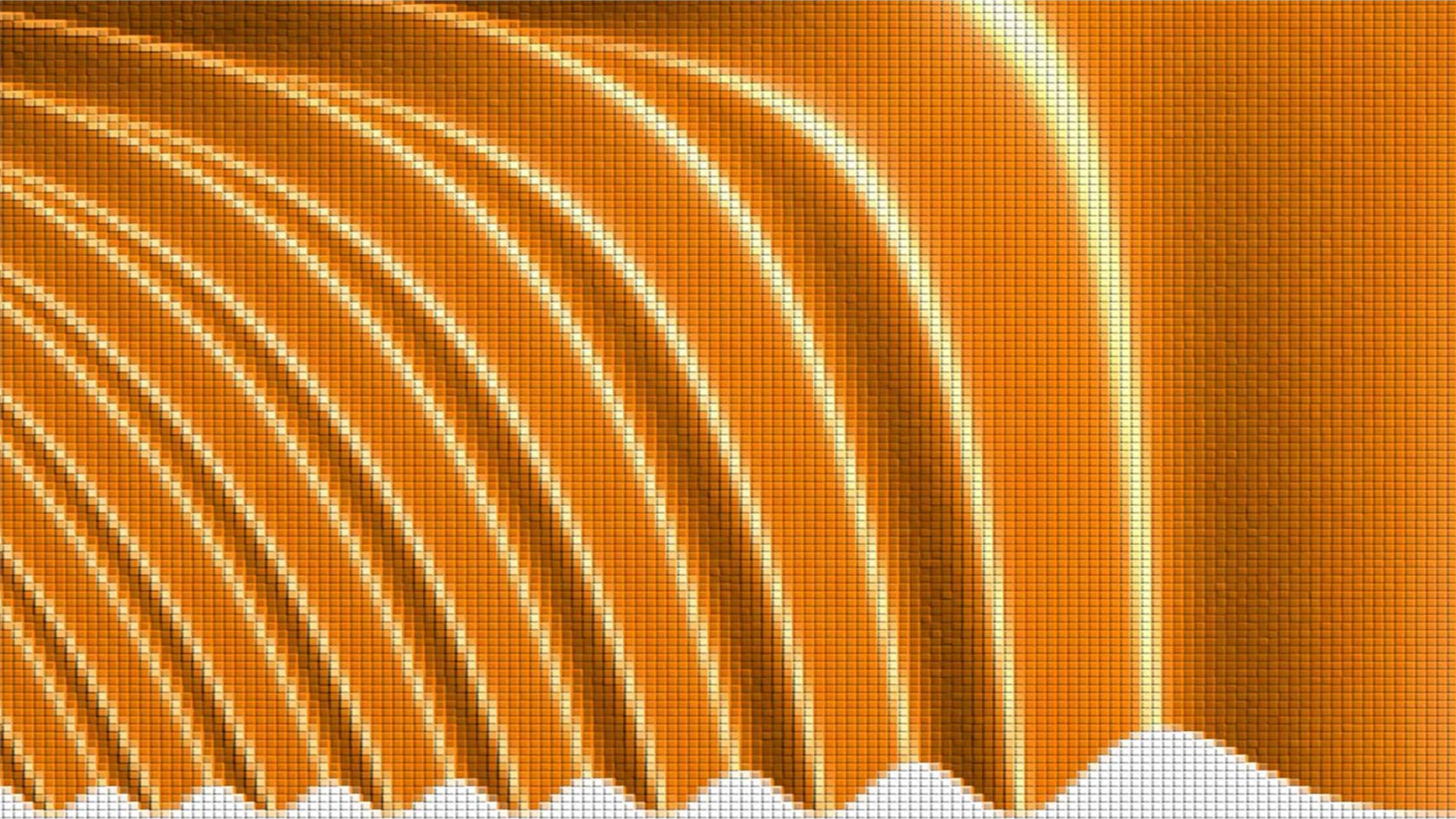
generates a matrix

Outer product

$$|g\rangle\langle f| = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix} \begin{bmatrix} c_1^* & c_2^* & c_3^* & \cdots \end{bmatrix} = \begin{bmatrix} d_1c_1^* & d_1c_2^* & d_1c_3^* & \cdots \\ d_2c_1^* & d_2c_2^* & d_2c_3^* & \cdots \\ d_3c_1^* & d_3c_2^* & d_3c_3^* & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

The specific summation $\hat{A} \equiv \sum_{i,j} A_{ij} |\psi_i\rangle\langle\psi_j|$

- is actually, then, a sum of matrices
  - In the matrix $|\psi_i\rangle\langle\psi_j|$
    - the element in the ith row and the jth column is 1
      - All other elements are zero

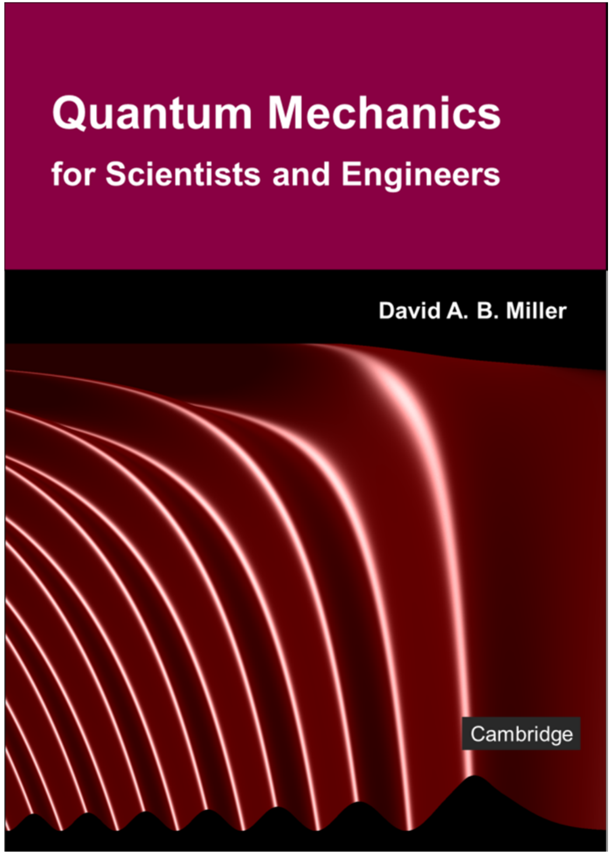


6.1 Types of linear operators

Slides: Video 6.1.3 The identity operator

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.8



Types of linear operators

The identity operator

Quantum mechanics for scientists and engineers

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Identity operator

The identity operator $\hat{I}$ is the operator that

- when it operates on a vector (function)
  - leaves it unchanged

In matrix form, the identity operator is

$$\hat{I} = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

In bra-ket form

- the identity operator can be written
  - where the $|\psi_i\rangle$
    - form a complete basis for the space

$$\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$$

Identity operator - proof

For an arbitrary function $|f\rangle = \sum_i c_i |\psi_i\rangle$ we know $c_m = \langle\psi_m|f\rangle$

so $|f\rangle = \sum_i \langle\psi_i|f\rangle|\psi_i\rangle$

Now, with our proposed form $\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$

then $\hat{I}|f\rangle = \sum_i |\psi_i\rangle\langle\psi_i|f\rangle$

But $\langle\psi_i|f\rangle$ is just a number

and so it can be moved in the product

Hence $\hat{I}|f\rangle = \sum_i \langle\psi_i|f\rangle|\psi_i\rangle$

and hence, using $|f\rangle = \sum_i \langle\psi_i|f\rangle|\psi_i\rangle$, $\hat{I}|f\rangle = |f\rangle$

Identity operator

The statement $\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$

is trivial if $|\psi_i\rangle$ is the basis used to represent the space

Then

$$|\psi_1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix} \text{ so that } |\psi_1\rangle\langle\psi_1| = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Identity operator

Similarly

$$|\psi_2\rangle\langle\psi_2| = \begin{bmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \qquad |\psi_3\rangle\langle\psi_3| = \begin{bmatrix} 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

so

$$\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i| = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Identity operator

Note, however, that $\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$

even if the basis being used is not the set $|\psi_i\rangle$

Then some specific $|\psi_i\rangle$

is not a vector with an ith element of 1 and all other elements 0

and the matrix $|\psi_i\rangle\langle\psi_i|$ in general has possibly all of its elements non-zero

Nonetheless, the sum of all matrices $|\psi_i\rangle\langle\psi_i|$

still gives the identity matrix $\hat{I}$

We can use any convenient complete basis to write $\hat{I}$

Identity operator

The expression $\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$ has a simple vector meaning

In the expression $|f\rangle = \sum_i |\psi_i\rangle\langle\psi_i|f\rangle$

$\langle\psi_i|f\rangle$ is just the projection of $|f\rangle$ onto the $|\psi_i\rangle$ axis

so multiplying $|\psi_i\rangle$ by $\langle\psi_i|f\rangle$

that is, $\langle\psi_i|f\rangle|\psi_i\rangle = |\psi_i\rangle\langle\psi_i|f\rangle$

gives the vector component of $|f\rangle$ on the $|\psi_i\rangle$ axis

Provided the $|\psi_i\rangle$ form a complete set

adding these components up just reconstructs $|f\rangle$

Identity matrix in formal proofs

Since the identity matrix is the identity matrix

no matter what complete orthonormal basis we use to represent it

we can use the following tricks

First, we "insert" the identity matrix

in some basis

into an expression

Then, we rearrange the expression

Then, we find an identity matrix we can take out of the result

Proof that the trace is independent of the basis

Consider the sum, S

of the diagonal elements of an operator $\hat{A}$

on some complete orthonormal basis $|\psi_i\rangle$

$$S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle$$

Now suppose we have some other complete orthonormal basis $|\phi_m\rangle$

We can therefore also write the identity operator as

$$\hat{I} = \sum_m |\phi_m\rangle\langle\phi_m|$$

Proof that the trace is independent of the basis

In $S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle$

we can insert an identity operator just before $\hat{A}$

which makes no difference to the result

since $\hat{I}\hat{A} = \hat{A}$

so we have

$$S = \sum_i \langle \psi_i | \hat{I}\hat{A} | \psi_i \rangle = \sum_i \langle \psi_i | \left(\sum_m | \phi_m \rangle \langle \phi_m | \right) \hat{A} | \psi_i \rangle$$

Proof that the trace is independent of the basis

Rearranging $S = \sum_i \langle \psi_i | \hat{I}\hat{A} | \psi_i \rangle = \sum_i \langle \psi_i | \left(\sum_m | \phi_m \rangle \langle \phi_m | \right) \hat{A} | \psi_i \rangle$

reordering the sums $$S = \sum_m \sum_i \langle \psi_i | \phi_m \rangle \langle \phi_m | \hat{A} | \psi_i \rangle$$

moving the number $\langle \psi_i | \phi_m \rangle$ $$= \sum_m \sum_i \langle \phi_m | \hat{A} | \psi_i \rangle \langle \psi_i | \phi_m \rangle$$

moving a sum and associating $$= \sum_m \langle \phi_m | \hat{A} \left(\sum_i | \psi_i \rangle \langle \psi_i | \right) | \phi_m \rangle$$

recognizing $\hat{I} = \sum_i | \psi_i \rangle \langle \psi_i |$ $$= \sum_m \langle \phi_m | \hat{A}\hat{I} | \phi_m \rangle$$

Proof that the trace is independent of the basis

So, with now $S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle = \sum_m \langle \phi_m | \hat{A}\hat{I} | \phi_m \rangle$

the final step is to note that $\hat{A}\hat{I} = \hat{A}$

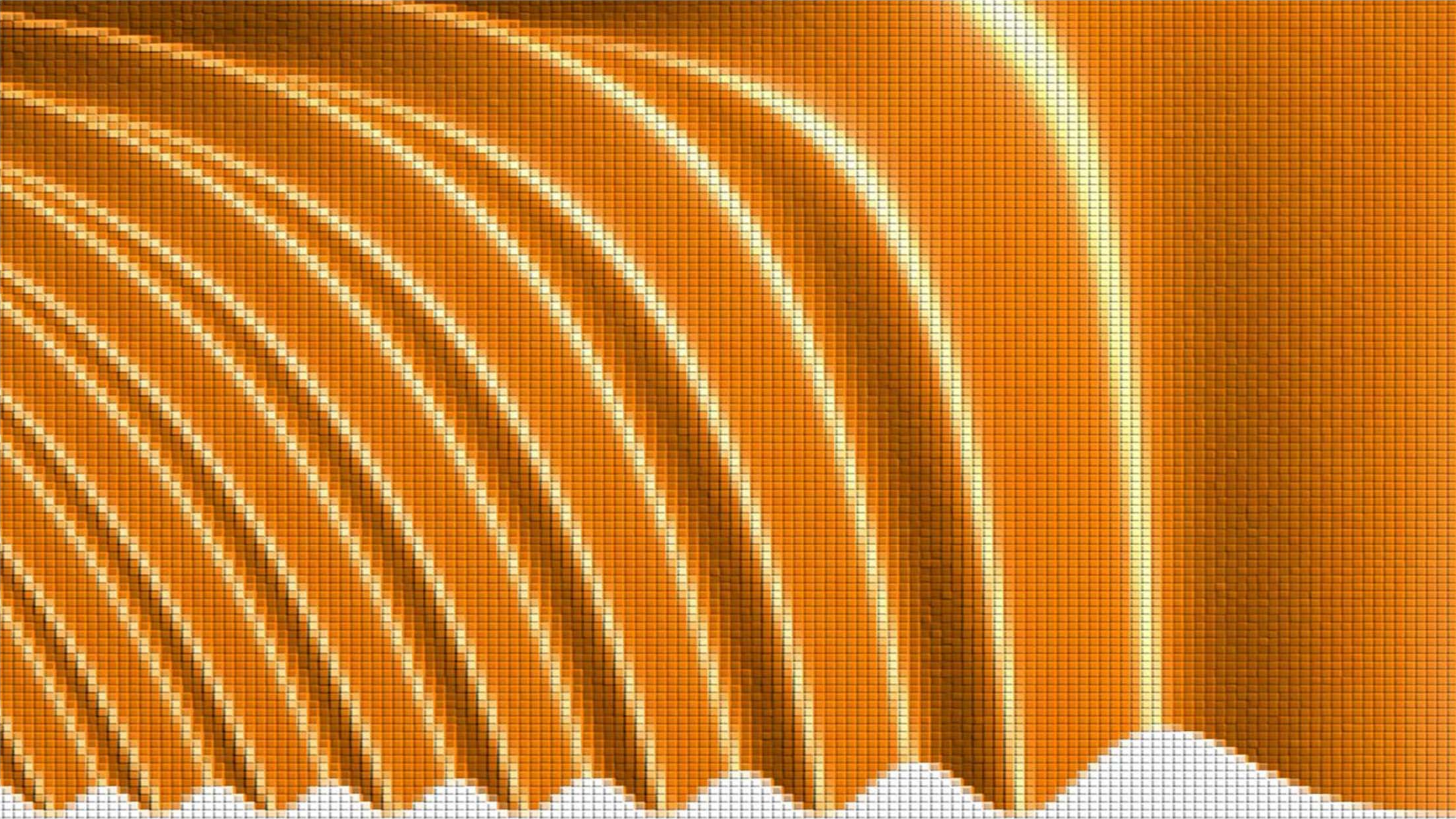
so $S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle = \sum_m \langle \phi_m | \hat{A} | \phi_m \rangle$

Hence the trace of an operator

the sum of the diagonal elements

is independent of the basis used to represent the operator

which is why the trace is a useful operator property

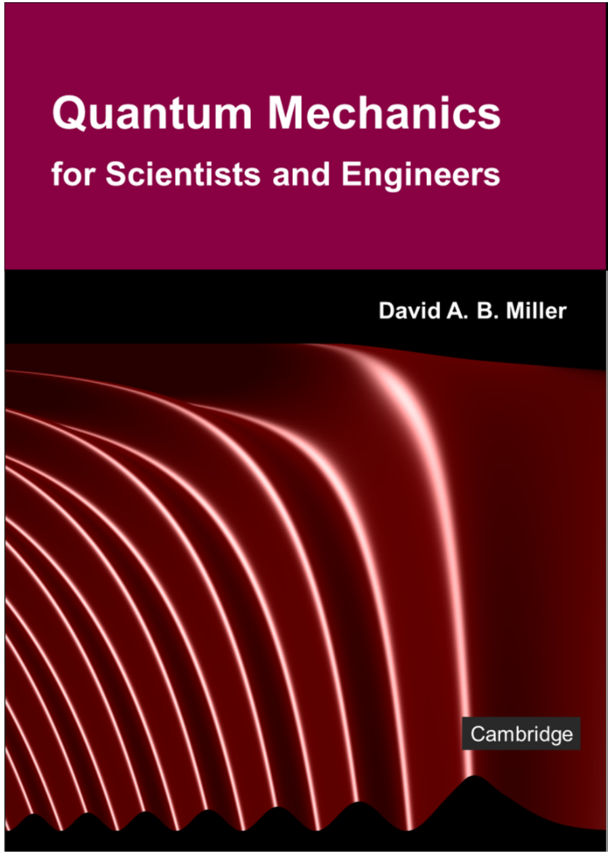


6.1 Types of linear operators

Slides: Video 6.1.5 Inverse and unitary operators

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 4.9 – 4.10 (up to "Changing the representation of vectors")



Types of linear operators

Inverse and unitary operators

Quantum mechanics for scientists and engineers

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Inverse operator

For an operator $\hat{A}$ operating on an arbitrary function $|f\rangle$

then the inverse operator, if it exists

is that operator $\hat{A}^{-1}$ such that

$$|f\rangle = \hat{A}^{-1}\hat{A}|f\rangle$$

Since the function $|f\rangle$ is arbitrary

we can therefore identify

$$\hat{A}^{-1}\hat{A} = \hat{I}$$

Since the operator can be represented by a matrix

finding the inverse of the operator reduces to

finding the inverse of a matrix

Projection operator

For example, the projection operator

$$\hat{P} = |f\rangle\langle f|$$

in general has no inverse

because it projects all input vectors

onto only one axis in the space

the one corresponding to the specific vector $|f\rangle$

Unitary operators

A unitary operator, $\hat{U}$, is one for which

$$\hat{U}^{-1} = \hat{U}^{\dagger}$$

that is, its inverse is its Hermitian adjoint

The Hermitian adjoint is formed by

reflecting on a -45° line and taking the complex conjugate

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots \\ u_{21} & u_{22} & u_{23} & \cdots \\ u_{31} & u_{32} & u_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}^{\dagger} = \begin{bmatrix} u_{11}^* & u_{21}^* & u_{31}^* & \cdots \\ u_{12}^* & u_{22}^* & u_{32}^* & \cdots \\ u_{13}^* & u_{23}^* & u_{33}^* & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Conservation of length for unitary operators

Note first that it can be shown generally that

for two matrices $\hat{A}$ and $\hat{B}$ that can be multiplied

$$\left(\hat{A}\hat{B}\right)^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$$

(this is easy to prove using the summation notation for matrix or vector multiplication)

That is, the Hermitian adjoint of the product is

the "flipped round" product of the Hermitian adjoints

Explicitly, for matrix-vector multiplication

$$\left(\hat{A}|h\rangle\right)^{\dagger} = \langle h|\hat{A}^{\dagger}$$

Conservation of length for unitary operators

Consider the unitary operator $\hat{U}$ and vectors $|f_{old}\rangle$ and $|g_{old}\rangle$

We form two new vectors by operating with $\hat{U}$

$$|f_{new}\rangle = \hat{U}|f_{old}\rangle \text{ and } |g_{new}\rangle = \hat{U}|g_{old}\rangle$$

Then $\langle g_{new}| = \langle g_{old}|\hat{U}^\dagger$

So $$\langle g_{new}|f_{new}\rangle = \langle g_{old}|\hat{U}^\dagger\hat{U}|f_{old}\rangle = \langle g_{old}|\hat{U}^{-1}\hat{U}|f_{old}\rangle = \langle g_{old}|\hat{I}|f_{old}\rangle$$
$$= \langle g_{old}|f_{old}\rangle$$

The unitary operation does not change the inner product

So, in particular $\langle f_{new}|f_{new}\rangle = \langle f_{old}|f_{old}\rangle$

the length of a vector is not changed by a unitary operator