

6.1 Types of linear operators

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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

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

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

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

Identity operator

Similarly

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

so

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

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 i th 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

