Unitary and Hermitian operators
Unitary operators to change representations of vectors

Suppose that we have a vector (function) \( |f_{\text{old}} \rangle \) that is represented when expressed as an expansion on the functions \( |\psi_n \rangle \) as the mathematical column vector

\[
|f_{\text{old}} \rangle = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}
\]

These numbers \( c_1, c_2, c_3, \ldots \) are the projections of \( |f_{\text{old}} \rangle \) on the orthogonal coordinate axes in the vector space labeled with \( |\psi_1 \rangle, |\psi_2 \rangle, |\psi_3 \rangle \ldots \)
Unitary operators to change representations of vectors

Suppose we want to represent this vector on a new set of orthogonal axes

which we will label $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ ...

Changing the axes

which is equivalent to changing the basis set of functions

does not change the vector we are representing

but it does change the column of numbers used to represent the vector
Unitary operators to change representations of vectors

For example, suppose the original vector $|f_{old}\rangle$
was actually the first basis vector in the old basis $|\psi_1\rangle$

Then in this new representation

the elements in the column of numbers

would be the projections of this vector

on the various new coordinate axes

each of which is simply $\langle \phi_m | \psi_1 \rangle$

So under this coordinate transformation

or change of basis

\[
\begin{bmatrix}
1 \\
0 \\
0 \\
\vdots
\end{bmatrix} \Rightarrow
\begin{bmatrix}
\langle \phi_1 | \psi_1 \rangle \\
\langle \phi_2 | \psi_1 \rangle \\
\langle \phi_3 | \psi_1 \rangle \\
\vdots
\end{bmatrix}
\]
Unitary operators to change representations of vectors

Writing similar transformations for each basis vector $|\psi_n\rangle$ we get the correct transformation if we define a matrix

\[
\hat{U} = \begin{bmatrix}
  u_{11} & u_{12} & u_{13} & \cdots \\
  u_{21} & u_{22} & u_{23} & \cdots \\
  u_{31} & u_{32} & u_{33} & \cdots \\
  \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
\]

where $u_{ij} = \langle \phi_i | \psi_j \rangle$

and we define our new column of numbers $|f_{\text{new}}\rangle$

\[
|f_{\text{new}}\rangle = \hat{U} |f_{\text{old}}\rangle
\]
Unitary operators to change representations of vectors

Note incidentally that here $|f_{\text{old}}\rangle$ and $|f_{\text{new}}\rangle$ are the same vector in the vector space.

Only the representation
- the coordinate axes
- and, consequently
- the column of numbers
  - that have changed
  - not the vector itself
Unitary operators to change representations of vectors

Now we can prove that $\hat{U}$ is unitary

Writing the matrix multiplication in its sum form

$$
(\hat{U}^{+}\hat{U})_{ij} = \sum_{m} u_{mi}^{*} u_{mj} = \sum_{m} \langle \phi_{m} | \psi_{i} \rangle^{*} \langle \phi_{m} | \psi_{j} \rangle = \sum_{m} \langle \psi_{i} | \phi_{m} \rangle \langle \phi_{m} | \psi_{j} \rangle
$$

$$
= \langle \psi_{i} \left| \left( \sum_{m} | \phi_{m} \rangle \langle \phi_{m} | \right) \right| \psi_{j} \rangle = \langle \psi_{i} | \hat{I} | \psi_{j} \rangle = \langle \psi_{i} | \psi_{j} \rangle = \delta_{ij}
$$

so $\hat{U}^{+}\hat{U} = \hat{I}$

hence $\hat{U}$ is unitary

since its Hermitian transpose is therefore its inverse
Unitary operators to change representations of vectors

Hence any change in basis can be implemented with a unitary operator.

We can also say that any such change in representation to a new orthonormal basis is a unitary transform.

Note also, incidentally, that so the mathematical order of this multiplication makes no difference.

\[ \hat{U} \hat{U}^\dagger = (\hat{U}^\dagger \hat{U})^\dagger = \hat{I}^\dagger = \hat{I} \]
Unitary operators to change representations of operators

Consider a number such as $\langle g | \hat{A} | f \rangle$
where vectors $|f\rangle$ and $|g\rangle$ and operator $\hat{A}$ are arbitrary.
This result should not depend on the coordinate system.
So the result in an “old” coordinate system
$\langle g_{old} | \hat{A}_{old} | f_{old} \rangle$
should be the same in a “new” coordinate system.
That is, we should have
$\langle g_{new} | \hat{A}_{new} | f_{new} \rangle = \langle g_{old} | \hat{A}_{old} | f_{old} \rangle$
Note the subscripts “new” and “old” refer to representations
not the vectors (or operators) themselves.
Which are not changed by change of representation.
Only the numbers that represent them are changed.
Unitary operators to change representations of operators

With unitary \( \hat{U} \) operator to go from “old” to “new” systems we can write

\[
\langle g_{\text{new}} | \hat{A}_{\text{new}} | f_{\text{new}} \rangle = (| g_{\text{new}} \rangle)^\dagger \hat{A}_{\text{new}} | f_{\text{new}} \rangle
\]

\[
= (\hat{U} | g_{\text{old}} \rangle)^\dagger \hat{A}_{\text{new}} (\hat{U} | f_{\text{old}} \rangle) = \langle g_{\text{old}} | \hat{U}^\dagger \hat{A}_{\text{new}} \hat{U} | f_{\text{old}} \rangle
\]

Since we believe also that \( \langle g_{\text{new}} | \hat{A}_{\text{new}} | f_{\text{new}} \rangle = \langle g_{\text{old}} | \hat{A}_{\text{old}} | f_{\text{old}} \rangle \) then we identify

\( \hat{A}_{\text{old}} = \hat{U}^\dagger \hat{A}_{\text{new}} \hat{U} \)

or since \( \hat{U} \hat{A}_{\text{old}} \hat{U}^\dagger = (\hat{U} \hat{U}^\dagger) \hat{A}_{\text{new}} (\hat{U} \hat{U}^\dagger) = \hat{A}_{\text{new}} \) then

\[
\hat{A}_{\text{new}} = \hat{U} \hat{A}_{\text{old}} \hat{U}^\dagger
\]
Unitary operators that change the state vector

For example, if the quantum mechanical state $|\psi\rangle$

is expanded on the basis $|\psi_n\rangle$ to give $|\psi\rangle = \sum_n a_n |\psi_n\rangle$

then $\sum_n |a_n|^2 = 1$

and if the particle is to be conserved

then this sum is retained as the quantum mechanical system evolves in time

But this is just the square of the vector length

Hence a unitary operator, which conserves length describes changes that conserve the particle
Unitary and Hermitian operators

Hermitian operators
Hermitian operators

A Hermitian operator is equal to its own Hermitian adjoint

\[ \hat{M}^\dagger = \hat{M} \]

Equivalently it is self-adjoint
Hermitian operators

In matrix terms, with

\[ \hat{M} = \begin{bmatrix}
  M_{11} & M_{12} & M_{13} & \cdots \\
  M_{21} & M_{22} & M_{23} & \cdots \\
  M_{31} & M_{32} & M_{33} & \cdots \\
  \vdots & \vdots & \vdots & \ddots
\end{bmatrix} \]

then

\[ \hat{M}^\dagger = \begin{bmatrix}
  M_{11}^* & M_{21}^* & M_{31}^* & \cdots \\
  M_{12}^* & M_{22}^* & M_{32}^* & \cdots \\
  M_{13}^* & M_{23}^* & M_{33}^* & \cdots \\
  \vdots & \vdots & \vdots & \ddots
\end{bmatrix} \]

so the Hermiticity implies \( M_{ij} = M_{ji}^* \) for all \( i \) and \( j \)

so, also

the diagonal elements of a Hermitian operator must be real
Hermitian operators

To understand Hermiticity in the most general sense consider

\[ \langle g | \hat{M} | f \rangle \]

for arbitrary \( |f\rangle \) and \( |g\rangle \) and some operator \( \hat{M} \)

We examine

\[ (\langle g | \hat{M} | f \rangle)\dagger \]

Since this is just a number

a “1 x 1” matrix

it is also true that

\[ (\langle g | \hat{M} | f \rangle)\dagger \equiv (\langle g | \hat{M} | f \rangle)^* \]
Hermitian operators

We can also analyze \((\langle g | \hat{M} | f \rangle)^\dagger\) using the rule \((\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger\)
for Hermitian adjoints of products

So \((\langle g | \hat{M} | f \rangle)^\star = (\langle g | \hat{M} | f \rangle)^\dagger = (\hat{M} | f \rangle)^\dagger (\langle g |)^\dagger = (| f \rangle)^\dagger \hat{M}^\dagger (\langle g |)^\dagger = \langle f | \hat{M}^\dagger | g \rangle\)

Hence, if \(\hat{M}\) is Hermitian, with therefore \(\hat{M}^\dagger = \hat{M}\)

then

\[
(\langle g | \hat{M} | f \rangle)^\star = \langle f | \hat{M} | g \rangle
\]

even if \(| f \rangle\) and \(| g \rangle\) are not orthogonal

This is the most general statement of Hermiticity
Hermitian operators

In integral form, for functions \( f(x) \) and \( g(x) \) the statement \( \left( \langle g \mid \hat{M} \mid f \rangle \right)^* = \langle f \mid \hat{M} \mid g \rangle \) can be written

\[
\int g^*(x) \hat{M} f(x) \, dx = \left[ \int f^*(x) \hat{M} g(x) \, dx \right]^*
\]

We can rewrite the right hand side using \( (ab)^* = a^*b^* \)

\[
\int g^*(x) \hat{M} f(x) \, dx = \int f(x) \{ \hat{M} g(x) \}^* \, dx
\]

and a simple rearrangement leads to

\[
\int g^*(x) \hat{M} f(x) \, dx = \int \{ \hat{M} g(x) \}^* f(x) \, dx
\]

which is a common statement of Hermiticity in integral form
Bra-ket and integral notations

Note that in the bra-ket notation
the operator can also be considered to operate to the left
\[ \langle g | \hat{A} | f \rangle \]
is just as meaningful a statement as \[ \hat{A} | f \rangle \]
and we can group the bra-ket multiplications as we wish
\[ \langle g | \hat{A} | f \rangle \equiv \left( \langle g | \hat{A} \rangle \right) | f \rangle \equiv \langle g | \hat{A} | f \rangle \]
Conventional operators in the notation used in integration
such as a differential operator, \( d/dx \)
do not have any meaning operating “to the left”
so Hermiticity in this notation is the less elegant form
\[
\int g^*(x) \hat{M} f(x) \, dx = \int \left\{ \hat{M} g(x) \right\}^* f(x) \, dx
\]
Reality of eigenvalues

Suppose $|\psi_n\rangle$ is a normalized eigenvector of the Hermitian operator $\hat{M}$ with eigenvalue $\mu_n$.

Then, by definition

$$\hat{M} |\psi_n\rangle = \mu_n |\psi_n\rangle$$

Therefore

$$\langle \psi_n | \hat{M} | \psi_n \rangle = \mu_n \langle \psi_n | \psi_n \rangle = \mu_n$$

But from the Hermiticity of $\hat{M}$ we know

$$\langle \psi_n | \hat{M} | \psi_n \rangle = (\langle \psi_n | \hat{M} | \psi_n \rangle)^* = \mu_n^*$$

and hence $\mu_n$ must be real.
Orthogonality of eigenfunctions for different eigenvalues

Trivially

$$0 = \langle \psi_m | \hat{M} | \psi_n \rangle - \langle \psi_m | \hat{M} | \psi_n \rangle$$

By associativity

$$0 = \left( \langle \psi_m | \hat{M} \rangle | \psi_n \rangle - \langle \psi_m | \hat{M} | \psi_n \rangle \right)$$

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

$$0 = \left( \langle \psi_m | \hat{M} \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \hat{M} | \psi_n \rangle$$

Using Hermiticity $$\hat{M} = \hat{M}^\dagger$$

$$0 = \left( \hat{M} | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \hat{M} | \psi_n \rangle$$

Using $$\hat{M} | \psi_n \rangle = \mu_n | \psi_n \rangle$$

$$0 = \left( \mu_m | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \mu_n | \psi_n \rangle$$

$$\mu_m$$ and $$\mu_n$$ are real numbers

$$0 = \mu_m (| \psi_m \rangle)^\dagger | \psi_n \rangle - \mu_n \langle \psi_m | \psi_n \rangle$$

Rearranging

$$0 = (\mu_m - \mu_n) \langle \psi_m | \psi_n \rangle$$

But $$\mu_m$$ and $$\mu_n$$ are different, so

$$0 = \langle \psi_m | \psi_n \rangle$$ i.e., orthogonality
Degeneracy

It is quite possible and common in symmetric problems to have more than one eigenfunction associated with a given eigenvalue. This situation is known as degeneracy.

It is provable that the number of such degenerate solutions for a given finite eigenvalue is itself finite.
Unitary and Hermitian operators

Matrix form of derivative operators
Matrix form of derivative operators

Returning to our original discussion of functions as vectors, we can postulate a form for the differential operator

\[
\frac{d}{dx} \equiv \begin{bmatrix}
... & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & 0 & ... \\
... & 0 & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & ... \\
... & 0 & 0 & \frac{1}{2\delta x} & ... \\
... & ... & & & &
\end{bmatrix}
\]

where we presume we can take the limit as \(\delta x \to 0\)
Matrix form of derivative operators

If we multiply the column vector whose elements are the values of the function then

\[
\begin{bmatrix}
\cdots \\
\cdots - \frac{1}{2\delta x} \\
\cdots 0 \\
\cdots 0 \\
\cdots - \frac{1}{2\delta x} \\
\cdots 0 \\
\cdots 0 \\
\cdots \frac{1}{2\delta x} \\
\cdots 0 \\
\cdots \frac{1}{2\delta x} \\
\cdots \vdots 
\end{bmatrix} \begin{bmatrix}
f(x_i - \delta x) \\
f(x_i) \\
f(x_i + \delta x) \\
f(x_i + 2\delta x) \\
\vdots
\end{bmatrix} = \begin{bmatrix}
\frac{f(x_i + \delta x) - f(x_i)}{2\delta x} \\
\frac{f(x_i + 2\delta x) - f(x_i)}{2\delta x} \\
\vdots
\end{bmatrix}
\]

where we are taking the limit as \( \delta x \rightarrow 0 \)

Hence we have a way of representing a derivative as a matrix
Matrix form of derivative operators

Note this matrix is antisymmetric in reflection about the diagonal and it is not Hermitian.

Indeed, somewhat surprisingly, \( \frac{d}{dx} \) is not Hermitian. By similar arguments, though, \( \frac{d^2}{dx^2} \) gives a symmetric matrix and is Hermitian.

\[
\frac{d}{dx} \equiv \begin{bmatrix}
\cdots & 0 & \frac{1}{2\delta x} & 0 \\
0 & \cdots & 0 & \frac{1}{2\delta x} \\
\frac{1}{2\delta x} & 0 & \cdots & 0 \\
\ddots & \ddots & \ddots & \ddots
\end{bmatrix}
\]
Matrix corresponding to multiplying by a function

We can formally “operate” on the function $f(x)$ by multiplying it by the function $V(x)$ to generate another function $g(x) = V(x)f(x)$.

Since $V(x)$ is performing the role of an operator, we can if we wish represent it as a (diagonal) matrix whose diagonal elements are the values of the function at each of the different points.

If $V(x)$ is real, then its matrix is Hermitian as required for $\hat{H}$.