Unitary and Hermitian operators

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Unitary operators to change representations of vectors

$$\left| f_{old} \right\rangle = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$$ With orthonormal basis function $\left| \psi_n \right\rangle$

$$\left| f_{new} \right\rangle = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix}$$ With new orthonormal basis function $\left| \phi_m \right\rangle$

Coordinate transform 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 $u_{ij} = \left\langle \phi_i \middle| \psi_j \right\rangle$

$$\left| f_{new} \right\rangle = \hat{U} \left| f_{old} \right\rangle$$

Unitary operators to change representations of vectors

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- prove that is unitary

$$\left(\hat{U}^{\dagger}\hat{U}\right)_{ij} = \sum_{m} u_{mi}^{*} u_{mj} = \sum_{m} \langle \phi_m | \psi_i \rangle^{*} \langle \phi_m | \psi_j \rangle = \sum_{m} \langle \psi_i | \phi_m \rangle \langle \phi_m | \psi_j \rangle$$

$$= \langle \psi_i | \left(\sum_{m} | \phi_m \rangle \langle \phi_m | \right) | \psi_j \rangle = \langle \psi_i | \hat{I} | \psi_j \rangle = \langle \psi_i | \psi_j \rangle = \delta_{ij}$$

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

- Hence unitary operator $\hat{U}$ is unitary since its Hermitian transpose is its inverse
- 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

Unitary operators to change representations of operators

Consider a number such as $\langle g | \hat{A} | f \rangle$

With unitary $\hat{U}$ operator to go from "old" to "new" systems

we can write $\langle g_{new} | \hat{A}_{new} | f_{new} \rangle = \left(| g_{new} \rangle \right)^{\dagger} \hat{A}_{new} | f_{new} \rangle$

$$= \left(\hat{U} | g_{old} \rangle \right)^{\dagger} \hat{A}_{new} \left(\hat{U} | f_{old} \rangle \right) = \langle g_{old} | \hat{U}^{\dagger} \hat{A}_{new} \hat{U} | f_{old} \rangle$$

Under the assumption $\langle g_{new} | \hat{A}_{new} | f_{new} \rangle = \langle g_{old} | \hat{A}_{old} | f_{old} \rangle$

Then we can derive $\hat{A}_{new}$

$$\hat{A}_{old} = \hat{U}^{\dagger} \hat{A}_{new} \hat{U}$$

$$\hat{U} \hat{A}_{old} \hat{U}^{\dagger} = \left(\hat{U} \hat{U}^{\dagger} \right) \hat{A}_{new} \left(\hat{U} \hat{U}^{\dagger} \right) = \hat{A}_{new}$$

Hermitian operators

In matrix terms, with

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

A Hermitian operator is equal to its own Hermitian adjoint

then

$$M_{ij} = M_{ji}^*$$

Hence, the diagonal elements of a Hermitian operator must be real

Hermitian operators

- statements

$\left(\langle g|\hat{M}|f\rangle\right)^{\dagger} \equiv \left(\langle g|\hat{M}|f\rangle\right)^{*}$ For arbitrary $|f\rangle$ and $|g\rangle$ Since result is just a value

So $\left(\langle g|\hat{M}|f\rangle\right)^{*} \equiv \left(\langle g|\hat{M}|f\rangle\right)^{\dagger} = \left(\hat{M}|f\rangle\right)^{\dagger}\left(\langle g|\right)^{\dagger} = \left(|f\rangle\right)^{\dagger}\hat{M}^{\dagger}\left(\langle g|\right)^{\dagger}$

$= \langle f|\hat{M}^{\dagger}|g\rangle$

In integral form

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

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

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

Hence,

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

Reality of eigenvalues

Suppose $|\psi_n\rangle$ is a normalized eigenvector of the Hermitian operator M with eigenvalue μ_n

Then, by the 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

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

and hence μ_n must be real

- Orthogonality of eigenfunctions for different eigenvalues

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

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

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

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

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

μ_m and μ_n are real numbers $\quad 0 = \mu_m\left(|\psi_m\rangle\right)^\dagger|\psi_n\rangle - \mu_n\langle\psi_m||\psi_n\rangle$

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

But μ_m and μ_n are different, so $0 = \langle\psi_m|\psi_n\rangle$ i.e., orthogonality

Matrix form of derivative operators

$$\begin{bmatrix} \ddots & & & & \\ \cdots -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & 0 \cdots & \\ \cdots 0 & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & \cdots \\ & & & & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ f(x_i - \delta x) \\ f(x_i) \\ f(x_i + \delta x) \\ f(x_i + 2\delta x) \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \frac{f(x_i + \delta_x) - f(x_i - \delta x)}{2\delta x} \\ \frac{f(x_i + 2\delta_x) - f(x_i)}{2\delta x} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \left.\frac{df}{dx}\right|_{x_i} \\ \left.\frac{df}{dx}\right|_{x_i + \delta x} \\ \vdots \end{bmatrix}$$

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

Indeed somewhat surprisingly d/dx is not Hermitian $\int f_n f_m' dx \neq (\int f_n' f_m dx)^*$

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 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 $\hat{H}$