

Physics 521, Quantum I

Lecture 3: Mathematical Foundations: Linear Operators

Given a Hilbert space \mathcal{H} (vector space of dimension d over complex \mathbb{C}) we define operators \hat{M} as maps of vectors in the space $\hat{M}: \mathcal{H} \rightarrow \mathcal{H}$, meaning $\hat{M}|u\rangle = |v\rangle$ for $|u\rangle, |v\rangle \in \mathcal{H}$.

In particular, we are interested in linear operators, meaning

$$\text{Given } |w\rangle = \alpha|u_1\rangle + \beta|u_2\rangle, \quad \alpha, \beta \in \mathbb{C}, \quad |u_1\rangle, |u_2\rangle \in \mathcal{H}$$

$$\text{If } \hat{M}|u_1\rangle = |v_1\rangle, \quad \hat{M}|u_2\rangle = |v_2\rangle$$

$$\text{Then } \boxed{\hat{M}|w\rangle = \alpha \hat{M}|u_1\rangle + \beta \hat{M}|u_2\rangle = \alpha|v_1\rangle + \beta|v_2\rangle}$$

Examples of linear operators

- Rotations on \mathbb{R}^3

$$\vec{w} = a\vec{u}_1 + b\vec{u}_2$$

$$\hat{R}: \vec{w} = c_1 \vec{u}_1 + c_2 \vec{u}_2$$

- Outer product: Let $\hat{E} = |\psi\rangle\langle\phi|$

$$\begin{aligned} \hat{E}|w\rangle &= \hat{E}(\alpha|u_1\rangle + \beta|u_2\rangle) = |\psi\rangle\langle\phi|(\alpha|u_1\rangle + \beta|u_2\rangle) = (\alpha\langle\phi|u_1\rangle + \beta\langle\phi|u_2\rangle)|\psi\rangle \\ &= \alpha \hat{E}|u_1\rangle + \beta \hat{E}|u_2\rangle \end{aligned}$$

Representations of operators as matrices

We have seen the vectors $|u\rangle \in \mathcal{H}$ are represented as column vectors in an orthonormal basis $\{|e_i\rangle \mid i=1, 2, \dots, d\}$, $|u\rangle = \sum_{i=1}^d u_i |e_i\rangle \stackrel{(lets)}{=} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_d \end{bmatrix}$. The dual vectors

(bras) are $\langle u| = \langle u|^T \stackrel{(lets)}{=} \sum_{i=1}^d u_i^* \langle e_i| = [u_1^* \ u_2^* \ \dots \ u_d^*] = \left(\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_d \end{bmatrix}^* \right)^T$ transpose

Conjugated row vector

$$\text{Now } |\psi\rangle = \hat{M}|\psi\rangle = \hat{M}\left(\sum_i u_i |e_i\rangle\right) = \sum_i u_i \hat{M}|e_i\rangle$$

$$\Rightarrow v_j = \langle e_j | \psi \rangle = \sum_i u_i \underbrace{\langle e_j | \hat{M} | e_i \rangle}_{\equiv M_{ji}}$$

R free index different from dummy

$$\Rightarrow v_j = \sum_i M_{ji} u_i$$

This is matrix multiplication

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{bmatrix} = \underbrace{\begin{bmatrix} M_{11} & M_{12} & \dots & M_{1d} \\ M_{21} & M_{22} & \dots & M_{2d} \\ \vdots & \vdots & & \vdots \\ M_{d1} & M_{d2} & \dots & M_{dd} \end{bmatrix}}_{\equiv \hat{M}} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_d \end{bmatrix} = \hat{M}|\psi\rangle$$

$$M_{ji} \equiv \langle e_j | \hat{M} | e_i \rangle \equiv \text{Matrix element } (\# \text{ complex})$$

row \rightarrow column

Using the resolution of the identity in a basis we can immediately form the representation:

$$\hat{1} = \sum_i |e_i\rangle \langle e_i|$$

$$\hat{M} = \hat{1} \hat{M} \hat{1} = \sum_{j,i} |e_j\rangle \underbrace{\langle e_j | \hat{M} | e_i \rangle}_{M_{ji}} \langle e_i| = \sum_{j,i} M_{ji} |e_j\rangle \langle e_i|$$

This is analogous to the dyadic expansion of tensors

$$\overleftarrow{T} = \sum_{j,i} T_{ij} \vec{e}_i \vec{e}_j$$

$$\overleftarrow{T} \cdot \vec{V} = \sum_{i,j} T_{ij} \vec{e}_i \cdot \vec{e}_j \cdot \vec{V} = \sum_{i,j} T_{ij} V_j \vec{e}_i$$

Note: $\sum_{j,i} M_{ji} |e_j\rangle \langle e_i|$ is an operator, independent of Basis

M_{ji} is a collection of #'s (matrix) depending on the basis

\hat{M} is a superposition of "transition" operator $\hat{E}_{ji} = |e_j\rangle\langle e_i|$

$$\Rightarrow \hat{M} = \sum M_{ji} \hat{E}_{ji}$$

Matrix representation of \hat{E}_{lk} in basis of $\{|e_i\rangle\}$

$$\langle e_j | \hat{E}_{lk} | e_i \rangle = \langle e_j | e_l \rangle \langle e_k | e_i \rangle = \delta_{jl} \delta_{ki}$$

$$\hat{E}_{lk} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \end{bmatrix} \text{ l^{th} row}$$

k^{th} column

$$\hat{M} = M_{11} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \end{bmatrix} + M_{12} \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \end{bmatrix} + \dots$$

$$= M_{11} |e_1\rangle\langle e_1| \qquad \qquad \qquad = M_{12} |e_2\rangle\langle e_2|$$

$$\text{Identity } \hat{1} = \sum_{ji} \langle e_j | \hat{1} | e_i \rangle |e_j\rangle\langle e_i| = \sum_{ji} \delta_{ji} |e_j\rangle\langle e_i| = \sum_i |e_i\rangle\langle e_i|$$

$$\hat{1} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \quad \begin{array}{l} \text{Diagonal matrix with 1's} \\ \text{on the diagonal + 0's elsewhere} \end{array}$$

Projection operator $|e_i\rangle\langle e_i| = 1$ on i^{th} row, i^{th} column

$$\Rightarrow \underbrace{\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}}_{\hat{1}} = \underbrace{\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}}_{= |e_1\rangle\langle e_1|} + \underbrace{\begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}}_{= |e_2\rangle\langle e_2|} + \dots + \underbrace{\begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}}_{= |e_d\rangle\langle e_d|}$$

Resolution of the identity

Inner & Outer Products : Matrix Representations

$$\langle u|v \rangle = [u_1^* \ u_2^* \ \dots \ u_d^*] \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{bmatrix} = \sum_i u_i^* v_i$$

$$|v\rangle\langle u| = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{bmatrix} [u_1^* \ u_2^* \ \dots \ u_d^*] = \begin{bmatrix} v_1 u_1^* & v_1 u_2^* & \dots & v_1 u_d^* \\ v_2 u_1^* & v_2 u_2^* & \dots & v_2 u_d^* \\ \vdots & \vdots & & \vdots \\ v_d u_1^* & \dots & v_d u_2^* & \dots & v_d u_d^* \end{bmatrix}$$

Important Operator / Matrix Manipulations. Let $M_{ij} = \langle e_i | \hat{M} | e_j \rangle$

- Transpose: $\hat{M}^T \Rightarrow (\hat{M}^T)_{ij} = M_{ji} = \langle e_j | \hat{M} | e_i \rangle$ (switch rows & column)
- Inverse: \hat{M}^{-1} defined $\hat{M}^{-1}\hat{M} = \hat{M}\hat{M}^{-1} = \hat{I}$ $\Rightarrow (\hat{M}^{-1})_{ij} (M_{jk}) = \delta_{ik}$
- Adjoint (Hermitian Conjugate) \hat{M}^+ (M "dagger") If $|w\rangle = \hat{M}|u\rangle$ then $\langle w| = \langle u|\hat{M}^+$
Note: $(\hat{M}^+)^+ = \hat{M} \Rightarrow$ If $\hat{M}^+|u\rangle = |w\rangle$ then $\langle w| = \langle u|\hat{M}$

$$\text{Now, } \langle v | \hat{M}^+ | u \rangle = \langle v | w \rangle \Rightarrow \langle v | w \rangle^* = \langle w | v \rangle = \langle u | M | v \rangle = \langle v | \hat{M}^+ | u \rangle^*$$

$$\Rightarrow \langle e_i | \hat{M}^+ | e_j \rangle = \langle e_j | \hat{M} | e_i \rangle^* \Rightarrow M_{ij}^+ = M_{ji}^* = (M_{ij}^T)^* \quad (\text{adjoint} = \text{conjugate-transpose})$$

As we will see, the adjoint of the matrix is like the complex conjugation of numbers

Important kinds of operators/matrices in quantum mechanics

- Hermition an operator for which $\hat{H}^\dagger = \hat{H}$ is said to be "Hermition" (self-adjoint)

This is the operator equivalent of a real number, $z^* = z$

If $\hat{A}^\dagger = -\hat{A}$, the operator is said to be "anti-Hermition" (sometimes "skew Hermition")

This is the operator equivalent of an imaginary number, $z^* = -z$

Any operator can be decomposed as $\hat{M} = \hat{H} + i\hat{A}$, like $z = x + iy$ (^{real + imag parts})

$$\hat{H} = \frac{\hat{M} + \hat{M}^+}{2} = \text{"Hermition part"}, \quad \hat{A} = \frac{\hat{M} - \hat{M}^+}{2i} = \text{"anti-Hermition part"}$$

- Unitary operators: \hat{U} defined s.t. $\hat{U}^\dagger = \hat{U}^{-1} \Rightarrow \hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \mathbb{1}$

This the operator equivalent of $z^*z = 1 \Rightarrow |z| = 1 \Rightarrow z = e^{i\theta}$

Multiplying by phase \rightarrow rotation of vector in complex plane $\Rightarrow \hat{U}$ is a "rotation in \mathcal{H} "

Unitary operators "preserve the inner product." That is, if $|u\rangle = \hat{U}|v\rangle$, $|v\rangle = \hat{U}|u\rangle$

$$\text{then } \langle u|\tilde{v}\rangle = \langle u|\hat{U}^\dagger \hat{U}|v\rangle = \langle u|\hat{1}|v\rangle = \langle u|v\rangle$$

Unitary operators map orthonormal basis to orthonormal basis.

Let $\{|e_i\rangle\}_{\text{basis}} = \text{orthonormal} \Rightarrow \{|\tilde{e}_i\rangle = \hat{U}|e_i\rangle\}$ is orthonormal \Rightarrow

$$\hat{U} = \sum_l |\tilde{e}_i\rangle \langle e_i| = \sum_{j,i} U_{ji} |e_j\rangle \langle e_i| \Rightarrow U_{ji} = \langle e_j|\tilde{e}_i\rangle$$

Columns & rows of U_{ji} are orthonormal

Change of basis, change of representation

Two different orthonormal basis lead to two different representations of the same vector or operator

Let $\{|e_i\rangle\}$ and $\{|\tilde{e}_i\rangle\}$ be orthonormal bases

$$\Rightarrow \hat{M} = \sum_{i,j} M_{ij} |e_i\rangle \langle e_j| = \sum_{k,l} \tilde{M}_{lk} |\tilde{e}_l\rangle \langle \tilde{e}_k|$$

where $M_{ij} = \langle e_i|\hat{M}|e_j\rangle$ and $\tilde{M}_{lk} = \langle \tilde{e}_l|\hat{M}|\tilde{e}_k\rangle$. How are these related?

Insert complete sets (resolution of the identity)

$$\tilde{M}_{lk} = \langle \tilde{e}_l | \hat{M} | \tilde{e}_k \rangle = \langle \tilde{e}_l | \left(\sum_i |e_i\rangle \langle e_i| \right) M \left(\sum_j |e_j\rangle \langle e_j| \right) | \tilde{e}_k \rangle$$

$$= \sum_{ij} \underbrace{\langle \tilde{e}_l | e_i \rangle}_{U_{il}^*} \underbrace{\langle e_i | M | e_j \rangle}_{M_{ij}} \underbrace{\langle e_j | \tilde{e}_k \rangle}_{U_{jk}} = \sum_{ij} (U^T)^* M_{ij} U_{jk}$$

$$\Rightarrow \tilde{M}_{lk} = \sum_{ij} (U^T)_{li} M_{ij} U_{jk} : \text{Unitary transformation}$$

A unitary transformation on a matrix is a special case of "similarity" transformation on a matrix $\tilde{M} = S^{-1} M S$, which changes arbitrary bases.

Note: Vector representation transformation: Let $|v\rangle = \sum_i v_i |e_i\rangle = \sum_j \tilde{v}_j |\tilde{e}_j\rangle$

$$\tilde{v}_j = \langle \tilde{e}_j | v \rangle = \sum_{ij} \langle \tilde{e}_j | e_i \rangle v_i = \sum_{ij} U_{ij}^* v_i = \sum_{ij} (U^T)_{ji} v_i$$

The matrix U_{ij} is a "passive" transformation on the coordinates

$(U|e_i\rangle = |\tilde{e}_i\rangle)$ is an "active" map on the basis vectors

Example: Pauli operators

The Pauli operators are familiar in the study of spin- $\frac{1}{2}$ particles, and as we will see, for a system described by a $d=2$ dimensional Hilbert space. The "standard basis" is spin-up and spin-down along the z -axis: $\{|+\rangle_z, |-\rangle_z\}$. In this basis

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$\hat{\sigma}_z$ is a diagonal matrix. This is because we have represented in the basis of its eigenvectors as we will review next lecture.

All of the Pauli matrices are Hermitian

$$\hat{\sigma}_x^+ = (\hat{\sigma}_x^*)^T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}^T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \hat{\sigma}_x$$

$$\hat{\sigma}_y^+ = (\hat{\sigma}_y^*)^T = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}^T = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \hat{\sigma}_y$$

$$\hat{\sigma}_z^+ = (\hat{\sigma}_z^*)^T = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}^T = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \hat{\sigma}_z$$

Interestingly, all the Pauli matrices are Unitary as well

$$\hat{\sigma}_x^+ \hat{\sigma}_x = \hat{\sigma}_x^2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = 1$$

$$\hat{\sigma}_y^+ \hat{\sigma}_y = \hat{\sigma}_y^2 = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = 1$$

$$\hat{\sigma}_z^+ \hat{\sigma}_z = \hat{\sigma}_z^2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = 1$$