Hilbert Space / Observables

Note Title

- A set of all vectors $|\alpha\rangle$ that are closed for the standard vector operations are called "vector space"
- A similar set of all wave functions defined over an interval $a \le x \le b$ is called a "Hilbert Space" for that particular interval.

- wave functions → square-integrable

$$\iff \int_a^b |f(x)|^2 dx < \infty$$

- Inner product of two functions $f(x)$ & $g(x)$

$$\langle f|g\rangle \equiv \int_a^b f(x)^* g(x)\, dx$$

[Compare for vectors

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \cdots$$]

- $\langle g|f\rangle = \langle f|g\rangle^*$
- $\langle f|f\rangle = \int_a^b |f(x)|^2 dx \geq 0$

- A set of functions is orthonormal if $\langle f_m|f_n\rangle = \delta_{mn}$,

- A set of functions is complete if any function in the Hilbert space can be expressed as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

$$\Rightarrow \quad c_n = \langle f_n | f \rangle$$

$$\left[\equiv \int_a^b f_n(x)^* f(x)\, dx \right]$$

$\boxed{\text{Ex.}}$ ① The set of energy eigenftns of the infinite square potential well over $[0, a]$.
② The set of energy eigenftns of the harmonic potential well over $[-\infty, \infty]$

Observables

- An "observable" operator Q always gives a real value for the measurement. That is

$$\langle Q \rangle = \langle Q \rangle^*$$

- This leads to the requirement that any observable operator should be hermitian (See the text book for proof)
- What does "hermitian" operator mean?

From Appendix A.6 ③

- A matrix T is called hermitian if

$$T^\dagger \equiv (\tilde{T}^*) = T$$

Ex)

$$T = \begin{pmatrix} 1 & i \\ i & 2 \end{pmatrix} \Rightarrow T^\dagger = \begin{pmatrix} 1 & -i \\ -i & 2 \end{pmatrix}$$

So this is not hermitian

$$T = \begin{pmatrix} 1 & i \\ -i & 2 \end{pmatrix} \Rightarrow T^\dagger = \begin{pmatrix} 1 & i \\ -i & 2 \end{pmatrix}$$

$\Rightarrow$ this is hermitian

$$T = \begin{pmatrix} 1 & i \\ 1 & 2 \end{pmatrix} \Rightarrow T^\dagger = \begin{pmatrix} 1 & 1 \\ -i & 2 \end{pmatrix}$$

$\Rightarrow$ this is not hermitian

[Here $T^\dagger$ is called the hermitian conjugate of T]

- For two matrices S & T

$$(S \cdot T)^\dagger = T^\dagger S^\dagger,$$

where $T^\dagger$ is called hermitian conjugate of T, and $(T^\dagger)^\dagger = T$

- For two vectors and a matrix

$$\vec{a}^\dagger T \cdot \vec{b} = (T^\dagger \vec{a})^\dagger \vec{b}$$

- In Dirac notations,

$$\vec{a}^{\dagger} T \vec{b} \Leftrightarrow \langle \alpha | T\beta \rangle$$

$$(T^{\dagger}\vec{a})^{\dagger} \vec{b} \Leftrightarrow \langle T^{\dagger}\alpha | \beta \rangle$$

so

$$\langle T^{\dagger}\alpha | \beta \rangle = \langle \alpha | T\beta \rangle$$

for any matrix (or operator) T

If T is a hermitian matrix

$$T^{\dagger} = T.$$

In other words $\langle T\alpha | \beta \rangle = \langle \alpha | T\beta \rangle$

$\boxed{\text{Ex.}}$ $|\alpha\rangle = \begin{pmatrix} i \\ 1 \end{pmatrix}$, $|\beta\rangle = \begin{pmatrix} 1 \\ i \end{pmatrix}$

Check for $T = \begin{pmatrix} 0 & i \\ 1 & 0 \end{pmatrix}$,

(non hermitian)

$$\langle \alpha | T\beta \rangle$$

$$= (-i \;\; 1)\begin{pmatrix} 0 & i \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ i \end{pmatrix} = (-i \;\; 1)\begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$= i + 1$$

$$\langle T\alpha | \beta \rangle = \left[\begin{pmatrix} 0 & i \\ 1 & 0 \end{pmatrix}\begin{pmatrix} i \\ 1 \end{pmatrix}\right]^{\dagger}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$= \begin{pmatrix} i \\ i \end{pmatrix}^{\dagger}\begin{pmatrix} 1 \\ i \end{pmatrix} = (-i, -i)\begin{pmatrix} 1 \\ i \end{pmatrix} = -i + 1$$

So $\langle \alpha | T\beta \rangle \neq \langle T\alpha | \beta \rangle$
for this case.

- But if we do $\langle T^{\dagger}\alpha | \beta \rangle$

$$= \left[\begin{pmatrix} 0 & 1 \\ -i & 0 \end{pmatrix} \begin{pmatrix} i \\ 1 \end{pmatrix} \right]^{\dagger} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$= \begin{bmatrix} 1 \\ 1 \end{bmatrix}^{\dagger} \begin{pmatrix} 1 \\ i \end{pmatrix} = (1 \;\; 1) \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$= 1 + i = \langle \alpha | T\beta \rangle .$$

- Now if we check for $T = \begin{pmatrix} 0 & i \\ -i & 1 \end{pmatrix}$, which is hermitian ($\because T^{\dagger} = T$)

$$\langle \alpha | T\beta \rangle = (-i \;\; 1) \begin{pmatrix} 0 & i \\ -i & 1 \end{pmatrix} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$= (-i \;\; 1) \begin{pmatrix} -1 \\ 0 \end{pmatrix} = \underline{i}$$

$$\langle T\alpha | \beta \rangle = \left[\begin{pmatrix} 0 & i \\ -i & 1 \end{pmatrix} \begin{pmatrix} i \\ 1 \end{pmatrix} \right]^{\dagger} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$= \begin{bmatrix} i \\ 2 \end{bmatrix}^{\dagger} \begin{pmatrix} 1 \\ i \end{pmatrix} = (-i \;\; 2) \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$= -i + 2i = \underline{i}$$

Thus $\langle \alpha | T\beta \rangle = \langle T\alpha | \beta \rangle$
as it should be for a hermitian matrix

* The most famous property of hermitian operator is that it's eigenvalues are always real.
This is also why all observables are represented by hermitian operators

$$\underset{\substack{\uparrow \\ \text{hermitian operator}}}{T}\,|\alpha\rangle = \underset{\substack{\uparrow \\ \text{eigenvalue} \\ \text{(real)}}}{\lambda}\,|\alpha\rangle$$

* Example of a non-matrix hermitian operator : $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$

Check if $\langle f | \hat{p} g \rangle = \langle \hat{p} f | g \rangle$

$$\langle f | \hat{p} g \rangle = \frac{\hbar}{i}\int_{-\infty}^{\infty} f^*(x) \frac{d}{dx} g(x)\, dx$$

$$= \frac{\hbar}{i}\left[\cancelto{0}{f^*(x) g(x) \Big|_{-\infty}^{\infty}} - \int_{-\infty}^{\infty} \frac{d f^*(x)}{dx} g(x)\, dx \right]$$

$$= \int_{-\infty}^{\infty} \left(\frac{\hbar}{i} \frac{d f(x)}{dx} \right)^* g(x)\, dx$$

$$= \int_{-\infty}^{\infty} (\hat{p} f(x))^* g(x)\, dx = \langle \hat{p} f | g \rangle$$

$\therefore$ $\hat{p}$ is an hermitian operator

Determinate States

* Measurement of an observable Q on a state $|\Psi\rangle$ is certain to yield the same value of q,
  $|\Psi\rangle$ is called a "determinate state", and this process can be mathematically expressed as

$$\hat{Q}|\Psi\rangle = q|\Psi\rangle$$

This type of equation is called eigenvalue equation. $|\Psi\rangle$ is an "eigenfunction" and "q" is the corresponding "eigenvalue"

* Determinate states of an observable $\hat{Q}$ are mathematically eigenfunctions of $\hat{Q}$

* Collection of all eigenvalues are called "spectrum"
* If two or more linearly independent eigenfunctions share the same eigenvalue the spectrum is said to be "degenerate".

* $\boxed{\text{Ex.}}$ $\hat{H}|\Psi\rangle = E|\Psi\rangle$
  E: eigenvalues of the hamiltonian $\hat{H}$
  $|\Psi\rangle$: stationary states = eigen ftns of $\hat{H}$.

$\boxed{\text{Ex}}$ Eigenvalue problem with matrices

$$T = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

Find its eigenvalues and eigenvectors.

$$T|\alpha\rangle = \lambda|\alpha\rangle, \qquad |\alpha\rangle \equiv \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

$\Rightarrow \quad (T - \lambda I)|\alpha\rangle = 0$

$\Rightarrow$ For $|\alpha\rangle$ to be non-zero, $\det(T - \lambda I) = 0$

$$\Rightarrow \det\left[\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} - \lambda\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right] = \det\begin{pmatrix} -\lambda & i \\ i & -\lambda \end{pmatrix}$$

$$= \lambda^2 - i^2 = (\lambda - i)(\lambda + i) = 0$$

$\therefore$ eigenvalues $\underline{\lambda = i, \ -i}$

eigenfunctions ?

For $\lambda = i$, $\begin{pmatrix} -i & i \\ i & -i \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = 0$

$$\Rightarrow \quad a_1 - a_2 = 0 \Rightarrow a_1 = a_2$$

$$\therefore \quad |\alpha\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix} a_1 = \underline{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}}$$

(normalized)

For $\lambda = -i$, $a_1 + a_2 = 0 \Rightarrow a_2 = -a_1$

$$|\alpha\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix} a_1 = \underline{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}}$$

$\boxed{\text{Ex}}$ Now non-matrix operator

$\hat{Q} \equiv i\frac{d}{d\phi}$, ϕ is the polar coordinate in 2D.

Find the eigenvalues and eigenfunctions, Check if it is hermitian

$\hat{Q}|\psi\rangle = \lambda|\psi\rangle$

with $|\psi\rangle = \psi(\phi)$

$i\frac{d}{d\phi}\psi(\phi) = \lambda\psi(\phi) \Rightarrow \frac{i}{\lambda}\frac{d\psi(\phi)}{d\psi} = d\phi$

$\Rightarrow \ln\psi(\phi) = -i\lambda\phi + \text{const}$

$\Rightarrow \psi(\theta) = Ae^{-i\lambda\phi}$

$\psi(0) = \psi(2\pi) \Rightarrow e^{-i\lambda 2\pi} = e^{0} = 1$

$\Rightarrow -i\lambda 2\pi = 2n\pi i \Rightarrow \lambda = -n$

$, n = 0, \pm 1, \pm 2, \ldots$

So eigenvalues, $\lambda =$ all integers

eigenfunctions, $\psi(\theta) = Ae^{-i\lambda\phi}$

$\langle f|\hat{Q}g\rangle =$

$$\int_0^{2\pi} f^*(\phi)\left(i\frac{d}{d\phi}\right)g(\phi)\,d\phi = i\left[f^*(\phi)g(\phi)\Big|_0^{2\pi} - \int_0^{2\pi}\frac{df^*(\phi)}{d\phi}g(\phi)\,d\phi\right]$$

$$= \int_0^{2\pi}\left(i\frac{df(\phi)}{d\phi}\right)^* g(\phi)\,d\phi$$

$= \langle\hat{Q}f|g\rangle$ $\therefore$ hermitian