

For example, in the infinite square well the set of functions that are normalizable i.e.

$$\int_0^a |f(x)|^2 dx < \infty,$$

define the "Hilbert space of the infinite square well". In general, in the $[a,b]$ interval:

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

We say the function is "square integrable"

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

This is the "inner product" of $f(x)$ with $g(x)$ (like dot product in 3D)

Properties of inner products:

$$\langle f|g \rangle^* = \left[\int_a^b f(x)^* g(x) dx \right]^* = \int_a^b g(x)^* f(x) dx = \langle g|f \rangle$$

Then: $\langle g|f \rangle = \langle f|g \rangle^*$

Prof recommendation: If in doubt, work with the explicit integrals as definition of inner product !

In particular: $\langle f|f \rangle = \int_a^b |f(x)|^2 dx$

It is real and non negative, justifying the **conjugation** in $f(x)$ in the definition of $\langle f|g \rangle$.
 $\langle f|f \rangle = 1$ means **normalized to 1**.

In this notation, then “orthonormality” of functions is written as:

$$\langle f_m | f_n \rangle = \delta_{mn}$$

“Completeness”: any function in the Hilbert space of the problem can be written as

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

$$|f\rangle = \sum_n c_n |f_n\rangle$$

$$\langle f_m | f \rangle = \sum_n c_n \underbrace{\langle f_m | f_n \rangle}_{\delta_{mn}}$$

Then, the coefficients are which is what we knew:

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

$$c_n \equiv \int_a^b f_n(x)^* f(x) dx$$

One last observation: **the Schwarz inequality**

In three dimensions, it is obvious:

$$(\mathbf{a} \cdot \mathbf{b})^2 = |\mathbf{a}|^2 |\mathbf{b}|^2 \cos^2 \phi \leq |\mathbf{a}|^2 |\mathbf{b}|^2$$

In N dimensions, it can be shown that:

$$|\langle f | g \rangle|^2 \leq \langle f | f \rangle \langle g | g \rangle$$

or, more explicitly, and taking square roots:

$$\left| \int_a^b f(x)^* g(x) dx \right| \leq \sqrt{\int_a^b |f(x)|^2 dx \int_a^b |g(x)|^2 dx}$$

Observables and Hermitian Operators

Expectation values of operators, such as $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, $\langle \hat{H} \rangle$, ... can be expressed in general as:

$$\langle \hat{Q} \rangle = \int \Psi^* \hat{Q} \Psi dx = \langle \Psi | \hat{Q} \Psi \rangle$$

where \hat{Q} is the \hat{x} , \hat{p} , \hat{H} , ... operator.

But if \hat{Q} is related with a **measurement**, physically we expect to obtain **real numbers**. Thus, for the operators of relevance:

$$\langle \hat{Q} \rangle = \langle \hat{Q} \rangle^*$$

Since $\langle \hat{Q} \rangle = \langle \hat{Q} \rangle^*$ means

$$\langle \Psi | \hat{Q} \Psi \rangle = \langle \Psi | \hat{Q} \Psi \rangle^* \quad \leftarrow \text{from physics common sense}$$

and since $\langle f | g \rangle^* = \langle g | f \rangle \quad \leftarrow \text{from math}$

$$(g = \hat{Q} \Psi, f = \Psi)$$

then $\langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$

Operators \hat{Q} that satisfy this property are called **Hermitian operators**.

Thus, observables are represented by Hermitian operators

Example 1: easy ... coordinate \hat{x} operator

$$\langle \hat{x} \rangle = \int \underbrace{\Psi^* \hat{x} \Psi}_{\langle \Psi | \hat{x} \Psi \rangle} dx = \int (x\Psi)^* \Psi dx = \langle \hat{x}\Psi | \Psi \rangle$$

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

Thus, \hat{x} is Hermitian

$(\hat{x})^2$ is also Hermitian, and in general potentials $V(\hat{x})$, like harmonic oscillator, are Hermitian.

Example 2: difficult ... momentum \hat{p} operator

$$\langle \hat{p} \rangle = \underbrace{\int \Psi^* \hat{p} \Psi dx}_{\langle \Psi | \hat{p} \Psi \rangle} = -i\hbar \int \Psi^* \frac{d}{dx} \Psi dx$$

$$\int_{-\infty}^{\infty} \Psi^* \frac{d}{dx} \Psi dx = \underbrace{\Psi^* \Psi \Big|_{-\infty}^{\infty}}_{=0} \ominus \int_{-\infty}^{\infty} \left(\frac{d}{dx} \Psi^* \right) \Psi dx$$

Thus, so far $\langle \Psi | \hat{p} \Psi \rangle = -i\hbar \int \Psi^* \frac{d}{dx} \Psi dx$

$$= (-i\hbar) \left(\ominus \int_{-\infty}^{\infty} \left(\frac{d}{dx} \Psi^* \right) \Psi dx \right) = \int_{-\infty}^{\infty} \left(-i\hbar \frac{d}{dx} \Psi \right)^* \Psi dx = \langle \hat{p} \Psi | \Psi \rangle$$

Because $\langle \Psi | \hat{p} \Psi \rangle = \langle \hat{p} \Psi | \Psi \rangle$
then, \hat{p} is a "Hermitian operator"

$-i \frac{d}{dx}$ is Hermitian (\hbar is just a constant)

$-\frac{d}{dx}$ is **not** Hermitian

$(-i \frac{d}{dx})^2$ is Hermitian

$\hat{H} = \hat{p}^2/2m + V(\hat{x})$ is Hermitian