2. Mathematical Tools
2.1 Vectors in 3D

$\underline{V} = (V_1, V_2, V_3)$

$\underline{W} = (W_1, W_2, W_3)$

Scalar product
(aka dot product or inner product)
$\langle \underline{V} \cdot \underline{W} \rangle = V_1 W_1 + V_2 W_2 + V_3 W_3$

Norm

$\|\underline{V}\| = \sqrt{\langle \underline{V} \cdot \underline{V} \rangle}$

$\|V\| \geq 0$

$\|V\| = 0 \Leftrightarrow \underline{V} = (0,0,0)$

Orthogonal
$\underline{V}$ and $\underline{W}$ are orthogonal if $\langle \underline{V}, \underline{W} \rangle = 0$, $\|\underline{V}\| = 1$, $\|\underline{W}\| = 1$.

Bases
$\underline{Z_1}, \underline{Z_2}, \underline{Z_3}$ are basis if any vector $\underline{V}$ can be written,
$\underline{V} = a\underline{Z_1} + b\underline{Z_2} + c\underline{Z_3}$
and the coefficients a, b and c are unique.
Furthermore, if $\underline{Z_1}$, $\underline{Z_2}$ and $\underline{Z_3}$ are orthogonal,

$a = \langle \underline{Z_1}, \underline{V} \rangle$

$b = \langle \underline{Z_2}, \underline{V} \rangle$

$c = \langle \underline{Z_3}, \underline{V} \rangle$

then,
$\underline{V} = \langle \underline{Z_1}, \underline{V} \rangle \underline{Z_1} + \langle \underline{Z_2}, \underline{V} \rangle \underline{Z_2} + \langle \underline{Z_3}, \underline{V} \rangle \underline{Z_3}$

Projections
$\underline{\tilde{V}} = \langle \underline{Z_1} . \underline{V} \rangle \underline{Z_1} + \langle \underline{Z_2} . \underline{V} \rangle \underline{Z_2}$
$\underline{\tilde{V}}$ is the projection of $\underline{V}$ onto the subspace spanned by $\underline{Z_1}$ and $\underline{Z_2}$.
(Basically, the projection of a 3D vector onto a 2D surface)

2.2 Functions as Vectors

$f(x)$: $\mathbb{R} \rightarrow \mathbb{C}$

$g(x)$: $\mathbb{R} \rightarrow \mathbb{C}$

Scalar Product
$\langle f(x), g(x) \rangle = \int_{-\infty}^{\infty} f^*(x) g(x) dx$

Property: $\langle f(x), g(x)\rangle^* = \langle g(x), f(x)\rangle$

Norm

$$\|f(x)\| = \sqrt{\langle f(x), f(x)\rangle} = \left[\int_{-\infty}^{\infty} f^*(x) f(x)\,dx\right]^{1/2} = \left[\int_{-\infty}^{\infty} |f(x)|^2\,dx\right]^{1/2}$$

Basis

If $f_1(x)$, $f_2(x)$ …, $f_N(x)$ are orthonormal basis functions, then any function $\psi(x)$:

$$\psi(x) = \sum_{i=1}^{N} a_i f_i(x) = \sum_{i=1}^{N} \langle f_i(x), \psi(x)\rangle f_i(x)$$

Projections

The projection of $\psi(x)$ onto the subspace spawned by f_1, f_2, f_3 is:

$$\psi'(x) = \langle f_1, \psi\rangle f_1 + \langle f_2, \psi\rangle f_2 + \langle f_3, \psi\rangle f_3$$

Continuous Bases

If $f_k(x)$ with $k \in \mathbb{R}$ is an orthonormal basis, if any function $\psi(x)$:

$$\psi(x) = \int_{-\infty}^{\infty} a_k f_k(x)\,dk$$

$$a_k = \langle f_k(x), \psi(x)\rangle = \int_{-\infty}^{\infty} f_k^*(x)\psi(x)\,dx$$

Example 1

$$f(p) = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$$

$$\psi(x) = \int_{-\infty}^{\infty} a_p \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$$

where:

$$a_p = \langle f_p(x), \psi(x)\rangle = \int_{-\infty}^{\infty} f_p^*(x)\psi(x)\,dx = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\psi(x)\,dx$$

Example 2

Dirac delta function $\delta(x - x')$

$$\psi(x) = \int_{-\infty}^{\infty} a_x \delta(x - x')\,dx'$$

$$a_x = \int_{-\infty}^{\infty} \delta(x - x')\psi(x)\,dx = \psi(x')$$

$$\psi(x) = \int_{-\infty}^{\infty} \psi(x')\delta(x - x')\,dx'$$

How to find $\|\psi\|^2$

Discrete case:

$$\|\psi\|^2 = \langle\psi,\psi\rangle = \left\langle \sum_{i=1}^{N} a_i f_i, \sum_{j=1}^{N} a_j f_j \right\rangle$$

$$= \sum_{i,j=1}^{N} a_i * a_j \left\langle f_i, f_j \right\rangle = \sum_{i,j=1}^{N} a_i * a_j \delta_{ij} = \sum_{i,j=1}^{N} a_i * a_j = \sum_{i=1}^{N} |a_i|^2$$

where $\left\langle f_i, f_j \right\rangle$ is orthonormal.

Continuous case:

$$\|\psi\|^2 = \langle\psi,\psi\rangle = \left\langle \int_{-\infty}^{\infty} a_k f_k dk, \int_{-\infty}^{\infty} a_{k'} f_{k'} dk' \right\rangle$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} a_k * a_{k'} \langle f_k, f_{k'} \rangle dk\, dk'$$

$$= \int_{\infty}^{\infty} |a_k|^2 dk$$

where $\left\langle f_k, f_{k'} \right\rangle = \delta_{kk'}$ i.e. is orthonormal.

Linear operators

These take the function as the argument, and give us another function.

$\hat{A}\psi(x) = \phi(x)$

Linear operators satisfy:

$\hat{A}[a\psi_{\prime} + b\psi_2] = a\hat{A}\psi_1 + b\hat{A}\psi_2$

where a and be are complex numbers $(a, b \in \mathbb{C})$

Expectation values

System in state ψ

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi(x) * \hat{A}\psi(x) dx = \left\langle \psi, \hat{A}\psi \right\rangle$$

Eigenfunctions and Eigenvalues of operators

$\psi(x)$ is an eigenfunction of $\hat{A}$ if:

i. $\psi(x) \equiv 0$
ii. $\hat{A}\psi = \lambda\psi$ where $\lambda \in \mathbb{C}$: eigenvalue.

The set of all the eigenvalues of $\hat{A}$ is called the spectrum of $\hat{A}$.

Properties:

i. $\hat{A}(\alpha\psi) = \lambda(\alpha\psi)$ $\alpha \in \mathbb{C}$

   ψ and $a\psi$ have the same eigenvalue.

ii. If

   $\hat{A}\varphi_1 = \lambda\varphi_1$

   $\hat{A}\varphi_2 = \sigma\varphi_2$

   and φ_1 and φ_2 are not multiple of each other, then λ is called a degenerate eigenvalue.

Any function of the form $\psi = a_1\varphi_1 + a_2\varphi_2$ is also an eigenfunction with eigenvalue λ. Then the subspace associated with λ is 2D.

Hermitian Operators

Hermitian operators satisfy $\int_{-\infty}^{\infty} \psi_1(x)^* \left(\hat{A}\psi_2(x)\right) dx = \int_{-\infty}^{\infty} \left(\hat{A}\psi_1(x)\right)^* \psi_2(x) dx$

$\left\langle \psi_1, \hat{A}\psi_2 \right\rangle = \left\langle \hat{A}\psi_1, \psi_2 \right\rangle$

Important properties of hermitian operators:

- All the eigenvalues are real
- Two eigenfunctions corresponding to two different eigenvalues are always orthogonal
- If an eigenvalue λ is degenerate with multiplicity p, we can find p orthogonal eigenfunctions associated to λ.

For a Hermitian operator we can find a set of orthogonal eigenfunctions.
Observables are always hermitian operators.

Matrix representation of operators

If ϕ_1, ϕ_2 and ϕ_3 are an orthogonal basis, we can associate to an operator $\hat{A}$ a matrix A with elements

$A_{ij} = \left\langle \phi_i, \hat{A}\phi_j \right\rangle$

$$A = \begin{pmatrix} \left\langle \phi_1, \hat{A}\phi_1 \right\rangle & \left\langle \phi_1, \hat{A}\phi_2 \right\rangle & \left\langle \phi_1, \hat{A}\phi_3 \right\rangle \\ \left\langle \phi_2, \hat{A}\phi_1 \right\rangle & \left\langle \phi_2, \hat{A}\phi_2 \right\rangle & \left\langle \phi_2, \hat{A}\phi_3 \right\rangle \\ \left\langle \phi_3, \hat{A}\phi_1 \right\rangle & \left\langle \phi_3, \hat{A}\phi_2 \right\rangle & \left\langle \phi_3, \hat{A}\phi_3 \right\rangle \end{pmatrix}$$

How to obtain $\hat{A}\psi$:

$$\psi = b_1\phi_1 + b_2\phi_2 + b_3\phi_3 \quad B = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

$A.B = C$

(Matrix multiplication)

$$C = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

→ $\xi = c_1\phi_1 + c_2\phi_2 + c_3\phi_3$

where $\xi = \hat{A}\psi$

Important prop:

If we know the action of an operator on a basis, then we know its' action on any function.

$\psi = b_1\phi_1 + b_2\phi_2 + b_3\phi_3$

$\hat{A}\psi = b_1\hat{A}\phi_1 + b_2\hat{A}\phi_2 + b_3\hat{A}\phi_3$

An operator is hermitian if its matrix representation satisfies:

$A = A^+$

where $A^+{}_{ij} = A_{ji}{}^*$

if $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$, then $A^+ = \begin{pmatrix} a_{11}{}^* & a_{12}{}^* \\ a_{21}{}^* & a_{22}{}^* \end{pmatrix}$