Some Necessary Math

You will learn that most operators in QM are linear (a few are antilinear) so what we need to review is about linear spaces.

I: Linear Space

A linear (or vector) space $\mathcal{V}$ over a Field F (real or complex numbers) has objects known as vectors or kets (this word is half of bracket; you will meet the other half shortly).

We will write kets (vectors) as $|v\rangle, |w\rangle, \ldots$

If $|v\rangle, |w\rangle \in \mathcal{V}$ then so do

(i) $a|v\rangle \quad a \in F$ Vectors can be scaled.

(ii) $|\phi\rangle = 0 \cdot |v\rangle$ Unique zero ket.

(iii) $|v\rangle + |w\rangle$ Vectors can be added

(iv) $|v\rangle + (-1)|v\rangle = |\phi\rangle \equiv 0$ No distinction between $|\phi\rangle$ and 0.

(1)

Later we will want to use $|0\rangle$ for a special state, the ground state.

All the objects we normally think of as vectors do indeed belong to vector spaces, but so do some others which we normally don't think of as vectors.

For example, the set of functions $f(x)$ $x \in [0,1]$ with $f(0) = f(1) = 0$ form a vector space with $F = R$ (real numbers).

II: Linear dependence: A set of n kets $|v_1\rangle \cdots |v_n\rangle$ with none of them being 0 is linearly dependent if we can find $a_1 \cdots a_n$ (not all $a_n = 0$) such that

$$\boxed{a_1|v_1\rangle + a_2|v_2\rangle + a_3|v_3\rangle + \cdots = 0} \quad (2)$$

$|v_i\rangle$ are linearly dependent.

Otherwise the kets are linearly independent.

A set of N linearly independent vectors $|v_i\rangle$ form a basis for $\mathcal{V}$ if any vector $|w\rangle$ can be expressed as a linear combination of $|v_i\rangle$

$$\boxed{|w\rangle = a_1|v_1\rangle + a_2|v_2\rangle + \cdots a_N|v_N\rangle} \quad (3)$$

Then the dimension of $\mathcal{V}$ is N.

The standard 3D space of position vectors is called $\mathbb{R}^3$ (real vector space of 3 dimensions).

We will be mostly concerned with complex linear spaces, the simplest of which is the complex plane $\mathbb{C}$

$\mathbb{C}$ just consists of all complex numbers. It is a linear space over the complex field, so complex numbers play a double role.

III: Dual Space

Now one can consider maps from one linear space to another.

Now consider a linear map from a linear space $\mathcal{V}$ to $\mathbb{C}$. It turns out that the set of such maps forms a linear space of the same dimension as $\mathcal{V}$. This space is the dual space of $\mathcal{V}$ and is called $\bar{\mathcal{V}}$. Elements of $\bar{\mathcal{V}}$ are dual vectors.

Temporarily let us denote elements of $\mathcal{V}$ by v and elements of $\bar{\mathcal{V}}$ by $\bar{v}$.

$$\boxed{\begin{gathered}\bar{v}(v) = z \in \mathbb{C} \\ \bar{v}(a v_1 + b v_2) = a\,\bar{v}(v_1) + b\,\bar{v}(v_2)\end{gathered}} \quad (4)$$

linearity.

The linear structure of $\bar{\mathcal{V}}$ is evident by

$$\boxed{(a\bar{v}_1 + b\bar{v}_2)(v) = a\,\bar{v}_1(v) + b\,\bar{v}_2(v)} \quad (5)$$

There is a unique zero map which satisfies

$$\boxed{\bar{v}_0(v) = 0 \quad \forall\, v \in \mathcal{V}} \quad (6)$$

Clearly, once we know the action of $\bar{v}$ on a set of basis vectors we know its action on any vector of $\mathcal{V}$

You should realize that the dual space is defined automatically for any linear space.

IV: General linear Maps

Now linear maps from $\mathcal{V}$ can take you to any other linear space. We will find it particularly relevant to physics when the target space is also $\mathcal{V}$

A Linear operator $\mathbb{M}$ is a map from $\mathcal{V} \to \mathcal{V}$ which preserves linearity

$$\boxed{\begin{array}{ll} \text{If} \quad \mathbb{M}|v\rangle = |v'\rangle & \mathbb{M}|w\rangle = |w'\rangle \\ \text{then} \quad \mathbb{M}(a|v\rangle + b|w\rangle) = a|v'\rangle + b|w'\rangle \end{array}} \tag{.7}$$

Clearly, this forces $\mathbb{M}(|\phi\rangle) = |\phi\rangle \equiv 0$

V: Inner product & Norm

There is an additional structure that we construct in common vector spaces called the norm (magnitude)

The norm requires a particular mapping between $\mathcal{V}$ and $\overline{\mathcal{V}}$ which has to be put in by hand, and is not automatic.

Now, for usual geometric vectors, we have a notion of the dot product of vectors. The generalization of this to an arbitrary linear space is the inner product.

To specialize to what we need in QM we will work with the complex number field. So from now on a, b, c will be complex.

To define the inner product, for every ket $|v\rangle$ we define a "bra" $\langle v|$ (this is the other half of the word bracket). This is sometimes called the adjoint of $|v\rangle$ and is an antilinear map from $\mathcal{V} \to \overline{\mathcal{V}}$

$$\boxed{\begin{aligned} &(|v\rangle)^{\dagger} = \langle v| \qquad (|w\rangle)^{\dagger} = \langle w| \\ &\text{then} \qquad (a|v\rangle + b|w\rangle)^{\dagger} = a^{*}\langle v| + b^{*}\langle w| \end{aligned}} \quad (8)$$

where the $*$ denotes complex conjugation
Now the inner product has to obey three rules

$$\boxed{\begin{aligned} &(i) \quad \langle v|w\rangle = \langle w|v\rangle^{*} \\ &(ii) \quad \langle v|v\rangle \geq 0 \quad \text{and is zero iff} \quad |v\rangle = 0 \\ &(iii) \quad \langle u|(a|v\rangle + b|w\rangle) = a\langle u|v\rangle + b\langle u|w\rangle \end{aligned}} \quad (9)$$

Given some specific inner product we can always find, in an N-dimensional vector space, N orthonormal kets we will call $|i\rangle$
This is the Gram-Schmidt theorem.

$$\boxed{\begin{aligned}&\langle i|j\rangle = \delta_{ij} \text{ (Kronecker delta symbol)} \\ &\sum_{i=1}^{N} |i\rangle\langle i| = \mathbb{1} \quad \text{complete orthonormal basis}\end{aligned}} \quad (10)$$

VI: Row & column vectors, matrices

Then any ket $|\psi\rangle$ can be expanded as

$$\boxed{|\Psi\rangle = \sum_{i=1}^{N} \psi_i |i\rangle \qquad \text{where} \quad \psi_i = \langle i|\psi\rangle} \quad (11)$$

ψ_i are the components $\wedge$ $|\Psi\rangle$ in the basis $|i\rangle$

Now if $|\Phi\rangle = \sum_{i=1}^{N} \phi_i |i\rangle$ then $\langle\Phi| = \sum_{i=1}^{N} \phi_i^* \langle i|$

so $$\boxed{\langle\Phi|\Psi\rangle = \sum_{i,j=1}^{N} \phi_i^* \psi_j \langle i|j\rangle = \sum_{i=1}^{N} \phi_i^* \psi_i} \quad (12)$$

It is traditional to represent $|\psi\rangle$ as a column vector and $\langle\psi|$ as a row vector

$$\boxed{|\psi\rangle = \begin{bmatrix}\psi_1 \\ \psi_2 \\ \vdots \\ \psi_N\end{bmatrix} \qquad \langle\psi| = [\psi_1^*, \psi_2^*, \dots, \psi_N^*]} \quad (13)$$

This has the convenient feature that the inner product becomes a matrix multiplication between a row and a column

Back to linear operators. Once we have an orthonormal basis we can write $\mathbb{M}$ as a matrix.

Consider $\mathbb{M}|j\rangle$ where $|j\rangle$ is a basis ket. This is some ket of $\mathcal{V}$ and can thus be expanded in terms of the basis kets.

$$\boxed{\mathbb{M}|j\rangle = \sum_i M_{ij}\, |i\rangle.} \quad (14)$$

where

$$\boxed{\begin{aligned} M_{ij} &\equiv \text{matrix element of } \mathbb{M} \\ &= \langle i|\mathbb{M}|j\rangle \end{aligned}} \quad (15)$$

Once we know the matrix elements of $\mathbb{M}$ we can find its action on any ket $|\Psi\rangle$

$$\text{Let } |\Psi\rangle = \sum_{j=1}^{N} \psi_j |j\rangle \quad (16)$$

$$\mathbb{M}|\Psi\rangle = \sum_{j=1}^{N} \psi_j\, \mathbb{M}|j\rangle = \sum_{j=1}^{N} M_{ij}\psi_j\, |i\rangle$$

Therefore if $\boxed{|\Phi\rangle = \mathbb{M}|\Psi\rangle = \sum_{i=1}^{N} \phi_i |i\rangle}$ (17)

$$\phi_i = \sum_j M_{ij}\psi_j$$

or

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} & \cdots & M_{1N} \\ M_{21} & M_{22} & \cdots & M_{2N} \\ \vdots & & & \\ \vdots & & & \\ M_{N1} & \cdots & \cdots & M_{NN} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \\ \psi_N \end{bmatrix} \quad (18)$$

We will denote operators by $\mathbb{M}, \mathbb{O}$ etc while matrices will be M, O etc.

VII : Hermitian Adjoint

For a linear operator $\mathbb{M}$ the hermitian adjoint $\mathbb{M}^\dagger$ is defined by

$$\boxed{\langle \Phi | \mathbb{M} \Psi \rangle = \langle \mathbb{M}^\dagger \Phi | \Psi \rangle} \quad (19)$$

Definition of $\mathbb{M}^\dagger$

The LHS is easily expanded as

$$\boxed{\langle \Phi | \mathbb{M} \Psi \rangle = \sum_{i,j} \phi_i^* M_{ij} \psi_j} \quad (20)$$

For the RHS we find

$$\boxed{\begin{aligned} \mathbb{M}^\dagger | \Phi \rangle &= | \mathbb{M}^\dagger \Phi \rangle = \sum_{i,j} (M^\dagger)_{ij} \phi_j | i \rangle \\ \text{So} \quad \langle \mathbb{M}^\dagger \Phi | &= \sum_{i,j} (M^\dagger)^*_{ij} \phi_j^* \langle i | \end{aligned}} \quad (21)$$

$$\Rightarrow \quad \boxed{\langle \mathbb{M}^\dagger \Phi | \Psi \rangle = \sum_{i,j} \phi_j^* (M^\dagger)^*_{ij} \psi_i} \quad (22)$$

Comparing we see that

$$(M^\dagger)^*_{ij} = (M)_{ji} \quad \text{or} \quad \boxed{(M^\dagger)_{ij} = M^*_{ji}} \quad (23)$$

The hermitian adjoint is represented by the conjugate transpose matrix

A linear operator is said to be hermitian if

$$\boxed{\mathbb{O} = \mathbb{O}^{+}} \quad (24)$$

definition of a hermitian operator

The importance of hermitian operators in QM comes from the fact that their eigenvalues are real, and every physical observable corresponds to a hermitian operator.

VIII: Transformations between orthonormal bases

There are an infinite number of ways to choose the axes in usual 3D space, all related by rotations. In an abstract linear space also one can choose different sets of orthonormal bases related by Unitary transformations

Suppose $|i\rangle$ $i=1,\cdots N$ is one orthonormal basis and $|\tilde{j}\rangle$ $j=1,\cdots N$ is another

$$\boxed{\langle i|j\rangle = \delta_{ij} \qquad \langle \tilde{i}|\tilde{j}\rangle = \delta_{ij}} \quad (25)$$

Since $|\tilde{i}\rangle$ is a ket in $\mathcal{V}$ we can expand it in the basis $|j\rangle$

$$\boxed{\begin{aligned} |\tilde{i}\rangle &= \sum_{\ell} U_{\ell i} |\ell\rangle \qquad U_{\ell i} = \langle \ell | \mathbb{U} | \tilde{i}\rangle \\ \langle \tilde{i}| &= \sum_{\ell} U^{*}_{\ell i} \langle \ell| \end{aligned}} \quad (26)$$

so
$$\boxed{\begin{aligned}\langle \tilde{i} | \tilde{j} \rangle &= \sum_{l,m} U^*_{li} U_{mj} \langle l | m \rangle \\ &= \sum_{l} U^*_{li} U_{lj} = \delta_{ij}\end{aligned}} \quad (27)$$

or
$$\boxed{\sum_l (U^{T*})_{il} U_{lj} = \sum_l (U^\dagger)_{il} U_{lj} = \delta_{ij}} \quad (28)$$

We can rewrite this as a matrix product. Defining the linear operator $\mathbb{1}$ (identity operator) with matrix elements δ_{ij} we get

$$\boxed{U^\dagger U = \mathbb{1}} \quad (29)$$

An important property a unitary transformation shares with geometric rotations is that it leaves inner products invariant.

$$\boxed{\langle \Phi | \Psi \rangle = \langle U\Phi | U\Psi \rangle} \quad (30)$$

From the definition of the hermitian adjoint

$$\langle U\Phi | U\Psi \rangle = \langle U^\dagger (U\Phi) | \Psi \rangle$$

$$= \langle U^\dagger U \Phi | \Psi \rangle = \langle \Phi | \Psi \rangle$$

Now consider how the matrices corresponding to linear operators transform under unitary changes of bases.

Say we start with an orthonormal basis $|i\rangle$ and transform to the new orthonormal basis $|\tilde{i}\rangle$

An operator $\mathbb{M}$ is characterized by its matrix elements

$$M_{ij} = \langle i | \mathbb{M} | j \rangle$$

In fact, we can write $\mathbb{M}$ as

$$\boxed{\mathbb{M} = \sum_{ij}{}' |i\rangle\langle i| \mathbb{M} |j\rangle\langle j|} \quad 31$$

However, the same operator can be expressed in the new basis

$$\mathbb{M} = \sum_{\tilde{i}\tilde{j}} |\tilde{i}\rangle\langle\tilde{i}| \mathbb{M} |\tilde{j}\rangle\langle\tilde{j}|$$

$$\boxed{\begin{aligned} \tilde{M}_{ij} &= \langle\tilde{i}| \mathbb{M} |\tilde{j}\rangle = \sum_{lm} U^*_{li} \langle l | \mathbb{M} | m\rangle U_{mj} \\ &= \sum_{lm} (U^\dagger)_{il} M_{lm} U_{mj} \end{aligned}} \quad 32$$

So as a matrix eq^n

$$\boxed{\tilde{M} = U^\dagger M U} \quad 33$$

Remember, the same operator is represented by different matrices in different bases.

IX: Eigenvalue problems:

Often in QM we want to find the eigenkets and eigenvalues of some linear operator. Usually (but not always) the operator is Hermitian, so let's focus on that case.

Consider some hermitian operator

$$\boxed{\mathbb{M}^\dagger = \mathbb{M}} \quad (34)$$

The eigenvalue problem is defined by

$$\boxed{\mathbb{M}|\psi_\alpha\rangle = \mu_\alpha |\psi_\alpha\rangle} \quad (35)$$

Let's first show that the eigenvalues have to be real. Take the adjoint of (35)

$$\boxed{\langle\psi_\alpha|\mathbb{M}^\dagger = \langle\psi_\alpha|\mathbb{M} = \mu_\alpha^* \langle\psi_\alpha|} \quad (36)$$

using the hermiticity of $\mathbb{M}$. From (35)

$$\langle\psi_\alpha|\mathbb{M}|\psi_\alpha\rangle = \mu_\alpha\langle\psi_\alpha|\psi_\alpha\rangle$$

From (36)

$$\langle\psi_\alpha|\mathbb{M}|\psi_\alpha\rangle = \mu_\alpha^* \langle\psi_\alpha|\psi_\alpha\rangle$$

So $\boxed{\mu_\alpha = \mu_\alpha^*}$ (37) A hermitian operator has real eigenvalues.

Now suppose we have two different eigenvalues $\mu_\alpha \neq \mu_\beta$

$$\mathbb{M}\,|\psi_\alpha\rangle = \mu_\alpha\,|\psi_\alpha\rangle \qquad \mathbb{M}\,|\psi_\beta\rangle = \mu_\beta\,|\psi_\beta\rangle$$

Carrying out the same steps with a few modifications we see

$$\boxed{\langle\psi_\alpha|\psi_\beta\rangle = 0 \quad \text{if} \quad \mu_\alpha \neq \mu_\beta} \quad (38)$$

The way to find the eigenvalues and eigenvectors is to first solve the characteristic eq^n

$$\boxed{\det\left[\mu\,\mathbb{1} - \mathbb{M}\right] = 0} \quad (39)$$

The roots of this polynomial give the eigenvalues μ_α. Once μ_α are known we solve (35) to get $|\psi_\alpha\rangle$

If all the eigenvalues are distinct, the spectrum of $\mathbb{M}$ is said to be nondegenerate. If some eigenvalues are identical there is a subspace of $\mathcal{V}$ which has that eigenvalue.

In either case we can find an orthonormal basis $|\alpha\rangle$ such that

$$\boxed{\mathbb{M}\,|\alpha\rangle = \mu_\alpha|\alpha\rangle \qquad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}} \quad (40)$$

An important way to write $\mathbb{M}$ in this basis is called the spectral representation of $\mathbb{M}$

$$\boxed{M = \sum_{\alpha} |\alpha\rangle \mu_\alpha \langle\alpha|} \quad (41)$$

You can easily check that this has the correct action on any ket.

In the spectral representation it is easy to write down any function of the linear operator M, which is also a linear operator

$$\boxed{\begin{aligned} M^n &= \sum_\alpha |\alpha\rangle (\mu_\alpha)^n \langle\alpha| \\ e^{M} &= \sum_\alpha |\alpha\rangle e^{\mu_\alpha} \langle\alpha| \end{aligned}} \quad (42)$$

etc.

Occasionally we will want the eigenvalues of unitary operators. It is easy to show that they have to be unimodular complex numbers.

$$U|\psi_\alpha\rangle = \lambda_\alpha |\psi_\alpha\rangle$$

$$\Rightarrow \langle\psi_\alpha| U^\dagger = \lambda_\alpha^* \langle\psi_\alpha|$$

$$\Rightarrow \langle\psi_\alpha| U^\dagger U |\psi_\alpha\rangle = |\lambda_\alpha|^2 \langle\psi_\alpha|\psi_\alpha\rangle$$

$$\Rightarrow \boxed{|\lambda_\alpha|^2 = 1} \quad (43) \text{ using } \quad U^\dagger U = \mathbb{1}$$

A Unitary operator has unimodular eigenvalues.