Advanced Quantum Mechanics

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1 Mathematical Tools of Quantum Mechanics. Postulates of Quantum Mechanics

1.1 Hilbert Spaces

Hilbert spaces, also known as **complex vector spaces**, are defined in **Definition 1.1**.

Definition 1.1. A Hilbert space $\mathcal{H}$ consists of a set of vectors ψ, ψ, χ, ... and a set of scalars a, b, c, ... which satisfy the following four properties:

1. $\mathcal{H}$ **is a linear space**[a].
2. $\mathcal{H}$ **has a defined scalar product that is strictly positive**. The scalar product of an element ψ with another element ϕ is in general a complex number, denoted by $(\psi,\ \phi)$. The scalar product satisfies the following properties[b]:

$$(\psi,\ \phi) = (\phi,\ \psi)^* \tag{1}$$

$$(\phi,\ a\psi_1 + b\psi_2) = a(\phi,\ \psi_1) + b(\phi,\ \psi_2) \tag{2}$$

$$(a\phi_1 + b\phi_2,\ \psi) = a^*(\phi_1,\ \psi) + b^*(\phi_2,\ \psi) \tag{3}$$

$$(\psi,\ \psi) = ||\psi||^2 \geq 0 \text{ (the equality holds only for } \psi = 0) \tag{4}$$

3. $\mathcal{H}$ **is separable**.
4. $\mathcal{H}$ **is complete**.

[a]See **Definition 2.1** for the definition of linear vector space.

[b]**Note:** Watch out for the order! Since the scalar product is a complex number, the quantity $(\psi,\ \phi) = \psi^*\phi$ is generall not equal to $(\phi,\ \psi) = \phi^*\psi$.

We should note that in a scalar product $(\phi,\ \psi)$, the second factor, ψ, belongs to the Hilbert space $\mathcal{H}$, while the first factor, ϕ, belongs to its dual Hilbert space $\mathcal{H}^*$[1]. The distinction between $\mathcal{H}$ and $\mathcal{H}^*$ is due to the fact that, as mentioned above, the scalar product is not commutative: $(\psi,\ \phi) \neq (\phi,\ \psi)$; the order matters!

1.2 The dual space

Given any Hilbert space $\mathcal{H}$, one can construct another complex vector space $\mathcal{H}^*$, called the **dual vector space**. It contains all the linear functionals in $\mathcal{H}$, which are a special kind of operator that maps all elements of $\mathcal{H}$ onto complex numbers[2]. In general, for an abstract vector space $\mathcal{H}$:

Definition 1.2. Given a Hilbert space $\mathcal{H}$, the dual space $\mathcal{H}^*$ is the vector space of all linear functionals in $\mathcal{H}$.

Therefore, all linear functionals $L : \mathcal{H} \to \mathbb{C}$ live in $\mathcal{H}^*$ $(L \in V^*)$.

The reason that the dual space is so interesting for quantum mechanics is that our goal as quantum physicists is to build a mathematical model for the real world, and in the end we want to be able to extract useful values and predictions from this model. For example, we may want to know the probability of getting a certain energy; or the average position we expect in a certain state. All these are scalar values, that we need to extract from a quantum state $|\psi\rangle$, so we know we will need a linear functional someplace or other!

[1]More on the dual space in the next section.

[2]See Appendix **Section 2.2** for more on linear functionals.

This may all sound really abstract at first glance, but hopefully it will become a lot clearer in the next section when we look at the **Dirac notation**.

1.3 Dirac Notation

In quantum mechanics, we use the Dirac notation to represent wave functions:

- We call the elements of $\mathcal{H}$ "ket" vectors, and we represent them as $|\psi\rangle \in \mathcal{H}$.
- We call the elements of $\mathcal{H}^*$ "bra" vectors, and we represent them as $\langle\phi| \in \mathcal{H}^*$.

Bra vectors are operators that linearly map elements of $\mathcal{H}$ into complex numbers:

$$\begin{array}{cccc} \langle\phi|: & \mathcal{H} & \rightarrow & \mathbb{C} \\ \langle\phi|: & |\psi\rangle & \rightarrow & \langle\phi\rangle\,\psi \end{array} \tag{5}$$

1.3.1 Inner product and bra-ket notation

Notice that, when we put a bra and a ket together ($\langle\phi|\,|\psi\rangle$), they look suspiciously like an inner product in this notation: $\langle\phi\rangle\,\psi$. If we go back at how our L_x operator in $\mathbb{R}^2$ acts on a column vector:

$$L_x \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix} = 1 \cdot a + 0 \cdot b = a \tag{6}$$

Notice that its action is the same as if we were taking the dot product with the x unit vector:

$$x \cdot \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix} = 1 \cdot a + 0 \cdot b = a \tag{7}$$

In fact, when a linear functional in $\mathbb{R}^n$ acts on any vector, it can be written equivalently as a dot product with the corresponding column vector:

$$L_x \vec{v} = L_x^T \cdot \vec{v} \tag{8}$$

This is actually a very general mathematical fact, rooted within something called the **Riesz Representation Theorem**:

Theorem 1.3. (Riesz Representation Theorem) For any linear functional L_ϕ, the action of L_ϕ is equivalent to taking the inner product with some unique vector $\vec{\phi}$.

In our example of L_x, we have that $\vec{\phi} = \vec{x} = [1\ 0]^T$:

$$L_x \vec{v} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cdot \vec{v} \tag{9}$$

This is the reason for the suggestive notation for bra vectors: they are operators whose action on a ket is mathematically equivalent to taking the inner product with said ket:

$$\langle\phi|\,|\psi\rangle = \langle\phi\rangle\,\psi \tag{10}$$

That is the power of bra-ket notation: it has the Riesz Representation Theorem baked right into it. Whatever you do, breaking apart inner products and putting together bras and kets, you will always have something that makes mathematical sense. Although bra and the inner product are two entities that are completely different mathematically, the bra-ket notation makes their connection completely seamless, thanks to the Riesz Representation Theorem.

1.3.2 Properties of bras and kets

Some properties that arise naturally from the Dirac notation:

$$\langle\psi\rangle\,\lambda_1\phi_1 + \lambda_2\phi_2 = \lambda_1\,\langle\psi\rangle\,\phi_1 + \lambda_2\,\langle\psi\rangle\,\phi_2 \tag{11}$$

$$\langle\lambda_1\psi + \lambda_2\psi_2\rangle\,\phi = \lambda_1^*\,\langle\psi_1\rangle\,\phi + \lambda_2^*\,\langle\psi_2\rangle\,\phi \tag{12}$$

$$\langle\psi\rangle\,\phi = \langle\phi\rangle\,\psi^* \tag{13}$$

$$\langle\psi\rangle\,\psi \text{ is real, positive and only zero if } |\psi\rangle = 0 \tag{14}$$

1.4 Linear operators

A linear map is defined as:

Definition 1.4. A linear map (or linear operator) is a mathematical entity A that associates a function with another function such that:

$$A(\lambda_1\psi_1 + \lambda_2\psi_2) = \lambda_1 A\psi_1 + \lambda_2 A\psi_2 \tag{15}$$

In the quantum mechanical context, we can see them as entities that transform a ket into another ket. Some example linear operators are:

- **Commutator:** The commutator of two operators A and B is defined as:

$$[A, B] \equiv AB - BA \tag{16}$$

  Two operators are said to commute if their commutator is equal to zero, and hence $AB = BA$. See **Section 2.5** to see an interesting application of commutator algebra for finding the uncertainty products of two operators.

- **Anti-commutator:** The anti-commutator of two operators A and B is defined as:

$$\{A, B\} \equiv AB + BA \tag{17}$$

- **Projector:** $P_\phi = |\phi\rangle\langle\phi|$. The projector operator P_ϕ acting on a ket $|\psi\rangle$ gives a new ket that is proportional to $|\phi\rangle$. The coefficient of proportionality is the scalar product $\langle\phi\rangle\,\psi$.[3]

- **Inverse:** assuming it exists, the inverse operator A^{-1} of the operator A, when applied to A, gives the identity operator. Also, A is the inverse of A^{-1}, so that $AA^{-1} = A^{-1}A = \mathbb{1}$.

- **Hermitian conjugation:** the hermitian conjugate (or adjoint) $A^\dagger$ of an operator A is obtained by interchanging the columns of the operator by its rows, and taking the complex conjugate of all elements. For example:

$$A = \begin{bmatrix} i & 1 \\ 3-i & -i \end{bmatrix} \rightarrow A^\dagger = \begin{bmatrix} -i & 3+i \\ 1 & i \end{bmatrix} \tag{18}$$

  Some properties of the adjoint are:

  a) $\left(A^\dagger\right)^\dagger = A$.

[3] *Proof:* $P_\phi\,|\psi\rangle = |\phi\rangle\,\langle\phi|\,|\psi\rangle = |\phi\rangle\,\langle\phi\rangle\,\psi = \langle\phi\rangle\,\psi\,|\phi\rangle$.

b) $(\lambda A)^\dagger = \lambda^* A^\dagger$.
c) $(A+B)^\dagger = A^\dagger + B^\dagger$.
d) $(AB)^\dagger = B^\dagger A^\dagger$.
e) $(|u\rangle \langle v|)^\dagger = |v\rangle \langle u|$.[4]

The adjoint of a bra is its ket, and the adjoint of a ket is its bra. To obtain the hermitian conjugate of an expression:

a) Replace constants with their complex conjugate: $\lambda \to \lambda^*$.
b) Replace operators with their Hermitian conjugates: $A \to A^\dagger$.
c) Replace kets with bras: $|\phi\rangle \to \langle\phi|$.
d) Replace bras with kets: $\langle\phi| \to |\phi\rangle$.
e) Reverse the order of factors: $A|\phi\rangle \to \langle\phi| A^\dagger$.

A special case of linear operators are **unitary operators**:

Definition 1.5. A linear operator U is said to be unitary if its inverse U^{-1} is equal to its adjoint $U^\dagger$, so that $U^{-1} = U^\dagger$ and $U^\dagger U = UU^\dagger = \mathbb{1}$.

Another special case are **Hermitian operators**:

Definition 1.6. An operator A is said to be Hermitian if $A^\dagger = A$.

and **anti-Hermitian operators**:

Definition 1.7. An operator A is said to be anti-Hermitian if $A^\dagger = -A$.

An example of a Hermitian operator is the projector operator, as $P_\phi^\dagger = (|\phi\rangle \langle\phi|)^\dagger = |\phi\rangle \langle\phi| = P_\phi$.

1.4.1 Expected value of an operator

In order to define the expected value of an operator, we first need to define the **matrix element**:

Definition 1.8. Let $|\psi\rangle$, $|\phi\rangle$ be two kets, we call the matrix element of an operator A between $|\psi\rangle$ and $|\phi\rangle$ the quantity $\langle\psi| (A|\phi\rangle)$.

Note that the matrix element of an operator A between $|\psi\rangle$ and $|\phi\rangle$ is a complex number, and it is equal to the scalar product of $|\psi\rangle$ with the ket $A|\phi\rangle$. If we now define the expected value of an operator:

Definition 1.9. The expected value $\langle A\rangle_\psi$ of A in the state $|\psi\rangle$ is defined as the matrix element of A between $|\psi\rangle$ and itself:

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle \tag{19}$$

It is easy to see that, if ψ is chosen to be an eigenvector of A, then the expected value of A in the state $|\psi\rangle$ is equal to the eigenvalue λ of A corresponding to the eigenvector $|\psi\rangle$:

$$\langle\psi|A|\psi\rangle = \langle\psi| (A|\psi\rangle) = \langle\psi| (\lambda|\psi\rangle) = \lambda \langle\psi|\psi\rangle = \lambda \tag{20}$$

[4] *Proof:* $\langle\phi| (|u\rangle \langle v|)^\dagger |\psi\rangle = [\langle\psi| (|u\rangle \langle v|) |\phi\rangle]^* = \langle\psi\rangle u^* \langle v\rangle \phi^* = \langle u\rangle \psi \langle\phi\rangle v = \langle\phi\rangle v \langle u\rangle \psi = \langle\phi| (|v\rangle \langle u|) |\psi\rangle$

This means that, for an arbitrary vector ϕ expressed as a linear combination of eigenvectors ψ_i of A:

$$|\phi\rangle = \sum_i c_i |\psi_i\rangle \tag{21}$$

we have:

$$\langle\phi|A|\phi\rangle = \sum_i\sum_j c_i^* c_j \langle\psi_i|A|\psi_j\rangle = \sum_i\sum_j c_i^* c_j \langle\psi_i|\lambda_j|\psi_j\rangle = \sum_i\sum_j c_i^* c_j \lambda_j \langle\psi_i|\psi_j\rangle =$$

$$= \sum_i\sum_j c_i^* c_j \lambda_j \delta_{ij} = \sum_i c_i^* c_i \lambda_i = \sum_i |c_i|^2 \lambda_i \tag{22}$$

1.5 Closure relation

For a set of vectors to form a basis of a Hilbert space $\mathcal{H}$, they must fulfil the **closure relation** (also known as the completeness relation). In simple terms, if the set of vectors fulfills the closure relation, it means that with those vectors you can reach all possible directions in $\mathcal{H}$, and any $|\psi\rangle \in \mathcal{H}$ is a linear combination of those basis vectors. In our general Hilbert space:

Definition 1.10. A set of vectors $\{|A_1\rangle, |A_2\rangle, ...\}$ in a Hilbert space $\mathcal{H}$ form a basis for $\mathcal{H}$ if and only if they fulfil the closure relation:

$$\mathbb{1} = \sum_i |A_i\rangle\langle A_i|. \tag{23}$$

Proof of this relation is given in **Section 2.4**.

1.6 Wave function space $\mathcal{F}$

The wave function in quantum mechanics is an object whose modulus squared is a probability density function. If we look back at **Definition 1.1**, we can see that, from a physical point of view, the set $\mathcal{H}$ is clearly too wide in scope for our purposes. We need to restrict it to a subset of $\mathcal{H}$ that is physically meaningful. This subset is called the **wave function space** $\mathcal{F}$, and it retains only the functions ψ of $\mathcal{H}$ which are everywhere defined, continuous, and infinitely differentiable. In addition, the functions of $\mathcal{F}$ must be normalizable by an arbitrary multiplicative constant in such a way that the area under the curve $|\psi|^2$ is exactly equal to 1.

1.7 Basis of the wave function space

If $\{|\psi_i\rangle\}$ is a basis for a Hilbert space $\mathcal{H}$ (in particular, the subset $\mathcal{F}$), we can expand every arbitrary vector $|\Psi\rangle$ according to this basis:

$$|\Psi\rangle = \sum_i c_i |\psi_i\rangle \tag{24}$$

so that we have[5]:

$$\langle\psi_i\rangle\,\Psi = \sum_j c_i \langle\psi_i\rangle\,\Psi = \sum_j c_i\delta_{ij} = c_i \tag{25}$$

The choice of basis is arbitrary, and depending on the choice we make, we obtain different representations of state space. There are many different representations, which often have to do with physical properties of the system.

[5] δ_{ij} is known as Kronecker's delta, and is equal to 1 if $i = j$ and 0 otherwise.

If you are familiar with basic quantum mechanics, you will probably have seen the position representation of the wave function, $\Psi(\vec{r})$. This representation of state space is particularly useful for working with position in a quantum system. However, it is not the *only* representation of state space that can have. What does this mean? Well, here, there is an important concept to understand, which is the difference between a vector and its representation: a vector is a mathematical entity that, once defined, is the same all the time, no matter where we look at it from or which basis we express it in. Its representation, however, may differ, depending on which basis we choose to represent it in. If the basis changes, the coordinates will also change, even though the vector is still the same.

For example, a vector $\vec{v}_B = (a, b)$ expressed in the basis $B = \{(1,0),\ (0,1)\}$ will change to $\vec{v}_{B'} = (b/2, a)$ $B' = \{(0,2),\ (1,0)\}$. The coordinates of the vector have changed, but we can see that both representations refer to the same vector:

$$\vec{v}_B = a \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{b}{2} \cdot \begin{pmatrix} 0 \\ 2 \end{pmatrix} + a \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \vec{v}_{B'} \tag{26}$$

Just as in this example, the position representation of the wave function vector space is only one of its many possible representations. The functions $\psi_i(\vec{r})$ form the basis for the position representation of state space. Other representations, like the momentum representation, can be useful in certain situations, as we will see later on.

1.8 Representations in state space

When studying quantum mechanical systems, we need a way to represent quantum states. We do that by choosing an orthonormal basis, either discrete or continuous, in the state space $\mathcal{F}$. Vectors and operators are then represented in this basis by numbers: components for the vectors and matrix elements for the operators.

As we mentioned before, the choice of a representation is, in principle, arbitrary. In fact, it depends on the particular problem being studied: in each case, one chooses the representation that leads to the simplest calculations.

Most useful bases come as eigenstates of some pertinent operator[6]. So far, we have mentioned the position and the momentum representation. These bases deal with the position and momentum operators, but you can think of many others. For example, the eigenstates of the Hamiltonian for some physical system are often used, especially when solving the Schrödinger equation. These might also be infinite dimensional but can be discrete, as opposed to the continuous bases of position and momentum.

1.8.1 General representation

For a general representation of state space (wave function space, $\mathcal{F}$), the elements of $\mathcal{F}$ are functions $\psi(\vec{\xi}),\ \phi(\vec{\xi})$, and the inner product in $\mathcal{F}$ is defined as:

$$\left(\phi(\vec{\xi}),\ \psi(\vec{\xi})\right) \equiv \int \phi^*(\vec{\xi})\psi(\vec{\xi})d\vec{\xi} \tag{27}$$

The length (norm) of a vector is given by:

$$\text{length}\left(\psi(\vec{\xi})\right) = \sqrt{\left(\psi(\vec{\xi}),\ \psi(\vec{\xi})\right)} = \sqrt{\int \psi^*(\vec{\xi})\psi(\vec{\xi})d\vec{\xi}} = \sqrt{\int \left|\psi(\vec{\xi})\right|^2 d\vec{\xi}} \tag{28}$$

[6]More on this lateradd link, but the idea is that, if we represent the state space in the basis of eigenstates (analogous to eigenvectors) of an operator, then that operator will be expressed in that basis as a diagonal matrix, where the elements of the diagonals are the eigenvalues of the operator. This makes calculations very easy.

As the vectors of the basis $\{\phi_i\}$ of $\mathcal{F}$ are orthonormal, we have that:

$$\left(\phi_i(\vec{\xi}),\ \phi_j(\vec{\xi})\right) = \delta_{ij} \tag{29}$$

1.8.2 Discrete orthonormal bases

A **discrete orthonormal basis** is defined as:

Definition 1.11. A countable set of functions $\{u_i\}$ is called orthonormal if:

$$\left(u_i(\vec{\xi}),\ u_j(\vec{\xi})\right) = \delta_{ij} \tag{30}$$

And it constitutes a basis for $\mathcal{F}$ if every function in $\mathcal{F}$ can be written as a linear combination of the functions of the basis in exactly one way:

$$\psi(\vec{\xi}) = \sum_i c_i u_i(\vec{\xi}) \tag{31}$$

with the coefficients being:

$$c_i = \left(u_i(\vec{\xi}),\ \psi(\vec{\xi})\right) = \int u_i^*(\vec{\xi})\psi(\vec{\xi})d\vec{\xi} \tag{32}$$

Note that, in a discrete orthonormal basis, all basis vectors u_i are elements belonging to $\mathcal{F}$. In other words, every basis vector u_i is a valid physical state for the system in the space $\mathcal{F}$. As we will see, this will *not* be the case for continuous orthonormal "bases".

For a discrete orthonormal basis, we can express the **scalar product in terms of the components** as:

$$\left(\phi(\vec{\xi}),\ \psi(\vec{\xi})\right) = \left(\sum_i b_i u_i(\vec{\xi}),\ \sum_j c_j u_j(\vec{\xi})\right) = \sum_{i,\ j} b_i^* c_j \left(u_i(\vec{\xi}),\ u_j(\vec{\xi})\right) = \sum_{i,\ j} b_i^* c_i \delta_{ij} = \sum_i b_i^* c_i \tag{33}$$

With a similar proof as in **Section 2.4**, we can find the closure relation for a discrete orthonormal basis:

$$\begin{aligned}\psi(\vec{\xi}) = \sum_i c_i u_i(\vec{\xi}) = \sum_i \left(u_i(\vec{\xi}),\ \psi(\vec{\xi})\right) u_i(\vec{\xi}) = \sum_i \left(\int u_i^*(\vec{\xi}')\psi(\vec{\xi}')d\vec{\xi}'\right) u_i(\vec{\xi}) = \\ = \int \left(\sum_i u_i^*(\vec{\xi}')u_i(\vec{\xi})\right)\psi(\vec{\xi}')d\vec{\xi}'\end{aligned} \tag{34}$$

Therefore, the term in the parenthesis must be equal to 1 for $\vec{\xi} = \vec{\xi}'$ and zero for every other case, so we obtain the **closure relation for a discrete orthonormal basis**[7]:

$$\sum_i u^*(\vec{\xi}')u_i(\vec{\xi}) = \delta(\vec{\xi} - \vec{\xi}') \tag{35}$$

1.8.3 Continuous orthonormal bases

A **continuous orthonormal basis** is defined as:

[7] $\delta(\vec{\xi} - \vec{\xi}')$ is known as Dirac's delta function, and it is equal to 1 if $\vec{\xi} = \vec{\xi}'$ and 0 otherwise. It can also be expressed as the integral $\delta(\vec{\xi} - \vec{\xi}') = \frac{1}{(2\pi)^3}\int e^{i\vec{k}\cdot(\vec{\xi}-\vec{\xi}')}d^3k$.

Definition 1.12. A continuous set of functions $\{\omega_\alpha\}$, labelled by a continuous index α, is called orthonormal if:

$$\Big(\omega_\alpha(\vec{\xi}),\ \omega_{\alpha'}(\vec{\xi})\Big) = \delta(\alpha-\alpha') \tag{36}$$

And it constitutes a basis for $\mathcal{F}$ if every function in $\mathcal{F}$ can be written as a linear combination of the functions of the basis in exactly one way:

$$\psi(\vec{\xi}) = \int c(\alpha)\omega_\alpha(\vec{\xi})d\alpha \tag{37}$$

with the continuous coefficient being:

$$c(\alpha) = \Big(\omega_\alpha(\vec{\xi}),\ \psi(\vec{\xi})\Big) = \int \omega_\alpha^*(\vec{\xi})\psi(\vec{\xi})d\vec{\xi} \tag{38}$$

Note that, $\langle\omega_\alpha(\vec{\xi})|\omega_{\alpha'}(\vec{\xi})\rangle = \delta(\alpha-\alpha')$ implies that the functions ω_α are not normaliseable[a], so these functions are *not* vectors in $\mathcal{F}$. Therefore, strictly speaking, they cannot be a basis for $\mathcal{F}$. In other words, basis vectors ω_α are *not* valid physical states for the system in the space $\mathcal{F}$. Rather, they are a mathematical tool that can help us to perform calculations in certain scenarios, and are formalised in what is known as a rigged Hilbert space[b]. However, we will still refer to them as "basis vectors" for simplicity.

[a] As $\langle\omega_\alpha(\vec{\xi})|\omega_{\alpha'}(\vec{\xi})\rangle = \delta(\alpha-\alpha')$ would imply that $\|\omega_\alpha\|^2 = \langle\omega_\alpha(\vec{\xi})|\omega_\alpha(\vec{\xi})\rangle = \delta(\alpha-\alpha) = \infty \neq 1$. So, it turns out that any basis in $\mathcal{F}$ has to be a discrete basis with an orthogonality condition expressed in terms of a Kronecker delta instead of a Dirac delta.

[b] See this and this post for more information.

For a continuous orthonormal basis, we can express the **scalar product in terms of the continuous coefficients** as:

$$\Big(\phi(\vec{\xi}),\ \psi(\vec{\xi})\Big) = \left(\int b(\alpha)\omega_\alpha(\vec{\xi})d\alpha,\ \int c(\alpha')\omega_{\alpha'}(\vec{\xi})d\alpha'\right) = \sum_{i,\ j} b_i^* c_j \Big(u_i(\vec{\xi}),\ u_j(\vec{\xi})\Big) =$$

$$= \int\left(\int b^*(\alpha)c(\alpha')(\omega_\alpha(\vec{\xi}),\omega_{\alpha'}(\vec{\xi}))d\alpha\right)d\alpha' = \int\left(\int b^*(\alpha)c(\alpha')\delta(\alpha-\alpha')d\alpha\right)d\alpha'$$

$$= \int b^*(\alpha)c(\alpha)d\alpha \tag{39}$$

With a similar proof as in **Section 2.4**, we can find the closure relation for a continuous orthonormal basis:

$$\psi(\vec{\xi}) = \int c(\alpha)\omega_\alpha(\vec{\xi})d\alpha = \int\Big(\omega_\alpha(\vec{\xi}),\ \psi(\vec{\xi})\Big)\omega_\alpha(\vec{\xi})d\alpha = \int\left(\int \omega_\alpha^*(\vec{\xi}')\psi(\vec{\xi}')d\vec{\xi}'\right)\omega_\alpha(\vec{\xi})d\alpha =$$

$$= \int\left(\int \omega_\alpha^*(\vec{\xi}')\omega_\alpha(\vec{\xi})d\alpha\right)\psi(\vec{\xi}')d\vec{\xi}' \tag{40}$$

Therefore, the term in the parenthesis must be equal to 1 for $\vec{\xi} = \vec{\xi}'$ and zero for every other case, so we obtain the **closure relation for a continuous orthonormal basis**:

$$\int \omega_\alpha^*(\vec{\xi}')\omega_\alpha(\vec{\xi})d\alpha = \Big(\omega_\alpha(\vec{\xi}'),\ \omega_\alpha(\vec{\xi})\Big) = \delta(\vec{\xi}-\vec{\xi}') \tag{41}$$

Fourier transform

Take the inverse fourier transform of the position wave function, for example:

$$\psi(\vec{r}) = \frac{1}{\sqrt{2\pi\hbar}}\int \overline{\psi}(\vec{p})e^{i\vec{p}\cdot\vec{r}/\hbar}d\vec{p} = \int \overline{\psi}(\vec{p})v_{\vec{p}}(\vec{r})d\vec{p}, \qquad v_{\vec{p}}(\vec{r}) = \frac{1}{\sqrt{2\pi\hbar}}e^{i\vec{p}\cdot\vec{r}/\hbar}\ \text{(plane wave)} \tag{42}$$

Notice that this is the same as:

$$\psi(\vec{\xi}) = \int c(\alpha)\omega_\alpha(\vec{\xi})d\alpha \tag{43}$$

where:

$$\alpha \to \vec{p} \text{ (continuous index)}, \quad c(\alpha) \to \overline{\psi}(\vec{p}), \quad \omega_\alpha(\vec{\xi}) \to v_{\vec{p}}(\vec{r}) \text{ (basis functions)} \tag{44}$$

And the "continuous coefficient" function $\overline{\psi}$ can be found as:

$$\overline{\psi}(\vec{p}) = (v_{\vec{p}}, \psi) = \int v^*_{\vec{p}}(\vec{r})\psi(\vec{r})d\vec{r} \tag{45}$$

It would seem that the set of uncountable $v_{\vec{p}}$ functions is a basis for $\mathcal{F}$, however, the integral of $\left|v_{\vec{p}}(\vec{r})\right|^2 = \frac{1}{2\pi\hbar}$ diverges, so $v_{\vec{p}}(\vec{r}) \notin \mathcal{F}$.

Delta function

In the same way, we can introduce the set of functions $\{\xi_{\vec{r}_0}(\vec{r})\}$ of $\vec{r}$, labelled by the continuous index $\vec{r}_0$ and defined as:

$$\xi_{\vec{r}_0}(\vec{r}) = \delta(\vec{r} - \vec{r}_0) \tag{46}$$

$\{\xi_{\vec{r}_0}(\vec{r})\}$ represents the set of delta functions centered at each of the points $\vec{r}_0$ of space. Clearly, $\xi_{\vec{r}_0}(\vec{r})$ is not square integrable, so $\xi_{\vec{r}_0}(\vec{r}) \notin \mathcal{F}$. Then, consider the relations:

$$\psi(\vec{r}) = \int \psi(\vec{r}_0)\delta(\vec{r} - \vec{r}_0)\ d^3r_0 = \int \psi(\vec{r}_0)\xi_{\vec{r}_0}(\vec{r})\ d^3r_0 \tag{47}$$

$$\psi(\vec{r}_0) = (\xi_{\vec{r}_0}, \psi) = \int \delta(\vec{r}_0 - \vec{r})\psi(\vec{r})\ d^3r = \int \xi^*_{\vec{r}_0}(\vec{r})\psi(\vec{r})\ d^3r \tag{48}$$

Equation 47 expresses the fact that every function $\psi(\vec{r}) \in \mathcal{F}$ can be expanded in terms of the $\xi_{\vec{r}_0}(\vec{r})$ functions in exactly one way. **Equation 48** shows that the value of the "continuous coefficient" corresponding to $\xi_{\vec{r}_0}(\vec{r})$ is preciesly $\psi(\vec{r}_0)$.

The usefulness of the continuous bases that we have just introduced is revealed more clearly in what follows. However, we must not lose sight of the following point: a physical state must always correspond to a square-integrable wave function. In no case can $v_{\vec{p}}(\vec{r})$ or $\xi_{\vec{r}_0}(\vec{r})$ represent the state of a particle. These functions are nothing more than intermediaries, very useful in calculations involving operations on the wave functions $\psi(\vec{r})$ which are used to describe a physical state.[8]

1.9 Matrix formulation of quantum mechanics

1.9.1 Matrix representation in discrete bases

Recall that, for a basis $\{|\phi_n\rangle\}$ of $\mathcal{F}$, we can write any $\psi \in \mathcal{F}$ as a linear combination of the basis vectors:

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle \tag{49}$$

where $c_n = \langle\phi_n|\psi\rangle$ represents the projection of $|\psi\rangle$ onto $|\phi_n\rangle$. So, within the basis $\{|\phi_n\rangle\}$, the ket $|\psi\rangle$ is represented by the set of its components, $c_1, c_2, ...,$ along $|\phi_1\rangle, |\phi_2\rangle, ...,$ respectively. Hence, we can write the ket $|\psi\rangle$ as a column vector:

$$|\psi\rangle \to \begin{pmatrix} \langle\phi_1|\psi\rangle \\ \langle\phi_2|\psi\rangle \\ \vdots \\ \langle\phi_n|\psi\rangle \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} \tag{50}$$

[8] aclarar

The bra $\langle\psi|$ is represented by the row vector:

$$\langle\psi| \to \big(\langle\psi|\phi_1\rangle \quad \langle\psi|\phi_2\rangle \quad \dots \quad \langle\psi|\phi_n\rangle\big) = \big(\langle\phi_1|\psi\rangle^* \quad \langle\phi_2|\psi\rangle^* \quad \dots \quad \langle\phi_n|\psi\rangle^*\big) = \big(c_1^* \quad c_2^* \quad \dots \quad c_n^*\big) \tag{51}$$

Just as kets and bras are respresented by column and row vectors, respectively, operators are represented by square matrices.

1.10 Eigenvalues and eigenvectors of an operator

We can define the **eigenvectors of an operator** as:

Definition 1.13. A state vector $|\psi\rangle$ is said to be an eigenvector (also called eigenket or eigenvector) of an operator A if it is a solution of the eigenvalue equation:

$$A\,|\psi\rangle = a\,|\psi\rangle \tag{52}$$

where a is a complex number, called an eigenvalue of A.

Some theorems regarding eigenvectors and eigenvalues are:

Theorem 1.14. The eigenvalues of the inverse A^{-1} of an operator A are the inverse (with respect to the multiplication, $1/a$) of the eigenvalues a of A. *Proof:*

$$A\,|\psi\rangle = a\,|\psi\rangle \to A^{-1}A\,|\psi\rangle = aA^{-1}\,|\psi\rangle \to |\psi\rangle = aA^{-1}\,|\psi\rangle \to A^{-1}\,|\psi\rangle = \frac{1}{a}\,|\psi\rangle \tag{53}$$

Theorem 1.15. For a Hermitian operator A, all of its eigenvalues are real and the eigenvectors corresponding to different eigenvalues are orthogonal[a].

[a] Proof in **Section 2.8**.

Theorem 1.16. If two Hermitian operators, A and B, commute and if A has no degenerate eigenvalue, then each eigenvector of A is also an eigenvector of B. In addition, we can construct a common orthonormal basis that is made of the joint eigenvectors of A and B[a].

[a] Proof in **Section 2.9**.

1.11 Position representation of state space

In the position representation, the basis consists of an infinite set of vectors $\{|\vec{r}\rangle\}$, which are eigenkets of the position operator $\vec{R}$:

$$\vec{R}\,|\vec{r}\rangle = \vec{r}\,|\vec{r}\rangle \tag{54}$$

where $\vec{r}$, the position vector, is the eigenvalue of the position operator $\vec{R}$. The orthonormality and completeness relations are given by:

$$\langle\vec{r}|\vec{r}\,'\rangle = \delta(\vec{r} - \vec{r}\,') \tag{55}$$

$$\int |\vec{r}\rangle\,\langle\vec{r}|\,d^3r = \mathbb{1} \tag{56}$$

In three dimensions, the delta function can be expressed as:

$$\delta(\vec{r} - \vec{r}\,') = \frac{1}{(2\pi)^3}\int e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}d^3k \tag{57}$$

So every state vector $|\psi\rangle$ can be expanded in terms of the position eigenkets $|\vec{r}\rangle$ as:

2 Appendix

2.1 Linear vector space

The definition of linear vector space is as follows:

Definition 2.1. A linear vector space consists of two sets of elements and two algebraic rules:

- A set of vectors $\psi,\ \phi,\ \chi,\ ...$ and a set of scalars $a,\ b,\ c,\ ....$
- A rule for adding vectors and a rule for multiplying vectors by scalars.

  a) **Addition:**
     - If ψ and ϕ are vectors (elements) of a space, their sum, $\psi + \phi$, is also a vector of the same space.
     - Commutativity: $\psi + \phi = \phi + \psi$.
     - Associativity: $(\psi + \phi) + \chi = \psi + (\phi + \chi)$.
     - Existence of a zero or neutral vector: for each vector ψ, there must exist a zero vector O such that: $\psi + O = O + \psi = \psi$.
     - Existence of a symmetric or inverse vector: each vector ψ must have a symmetric vector $(-\psi)$ such that $\psi + (-\psi) = (-\psi) + \psi = O$.

  b) **Multiplication:** The multiplication of vectors by scalars (scalars can be real or complex numbers) has these properties:
     - The product of a scalar with a vector gives another vector. In general, if ψ and ϕ are two vectors of the space, any linear combination $a\psi + b\phi$ is also a vector of the space, a and b being scalars.
     - Distributivity with respect to addition: a $(\psi+\phi) = a\psi + a\phi$, and $(a+b)\psi = a\psi + b\psi$.
     - Associativity with respect to multiplication of scalars: $a(b\psi) = (ab)\psi$
     - For each element ψ there must exist a unitary scalar I and a zero scalar "0" such that $I\psi = \psi I = \psi$ and $\psi 0 = 0\psi = O$. (2.3)

2.2 Linear functionals

In order to understand the mathematical background of the dual space, it is interesting to know the definitions of **linear maps** and **linear functionals**. We already defined linear operators in **Definition 1.4**. As for linear functionals:

Definition 2.2. A linear functional is a linear map L that associates a function with a scalar value, which may be real or complex.

An example of a linear functional could be the linear map $L_x : \mathbb{R}^2 \to \mathbb{R}$ that returns the x-coordinate of the vector it is given. For example:

$$L_x \begin{bmatrix} a \\ b \end{bmatrix} = a \tag{58}$$

In this case, L_x takes us from $\mathbb{R}^2$ to $\mathbb{R}^1$, so its matrix will be 1 by 2 in dimension:

$$L_x = \begin{bmatrix} 1 & 0 \end{bmatrix} \tag{59}$$

so that:

$$L_x \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix} = a \tag{60}$$

Taking a step back, we know that all linear functionals in $\mathbb{R}^2$ take us from $\mathbb{R}^2$ to $\mathbb{R}^1$. Therefore, by definition, all linear functionals in $\mathbb{R}^2$ are represented by 1×2 matrices. In other words, the set of all linear functionals in $\mathbb{R}^2$ consists of the set of all row matrices. More generally, the set of all linear functionals in $\mathbb{R}^n$ consists of the set of all $1 \times n$ row matrices. In fact, the set of all row matrices, much like column matrices, form their own vector space, which is known as the dual space[9].

2.3 Matrix element of an operator

The matrix element of an operator A is:

Definition 2.3. The matrix element of an operator A expressed in the basis $B = \{u_1, u_2, ...\}$ is defined as:

$$A_{ij} = \langle u_i | A | u_j \rangle \tag{61}$$

where u_i and u_j are the i-th and j-th vectors of the basis, respectively.

2.4 Proof of the Closure relation

The closure relation states that, for a set of vectors $\{|A_1\rangle, |A_2\rangle, ...\}$ to form a basis of a Hilbert space $\mathcal{H}$, they must fulfil the following relation:

If $B = \{\psi_1, \psi_2, ...\}$ is a basis for a Hilbert space $\mathcal{H}$, we can write any vector $|\psi\rangle \in \mathcal{H}$ as:

$$|\psi\rangle = \sum_i c_i |A_i\rangle \tag{62}$$

Where the coefficients are $c_i = \langle A_i \rangle \psi$[10]. If we substitute this expression:

$$|\psi\rangle = \sum_i \langle A_i \rangle \psi |A_i\rangle \tag{63}$$

As the coefficient is a complex number, we can move it to the end of the expression and separate the inner product:

$$|\psi\rangle = \sum_i |A_i\rangle \langle A_i| |\psi\rangle \tag{64}$$

As $|\psi\rangle$ is the same for every element of the sum, we can pull it out of the sum:

$$|\psi\rangle = \left(\sum_i |A_i\rangle \langle A_i| \right) |\psi\rangle \tag{65}$$

And it is now easy to see that this relation will hold if and only if the closure relation holds:

$$\sum_i |A_i\rangle \langle A_i| = \mathbb{1} \tag{66}$$

The inverse argument is easy to follow.

[9] See **Section 1.2** for more on the dual space

[10] *Proof:* As A_i form an orthonormal basis: $\langle A_i \rangle \psi = \langle A_i | \sum_j c_i |A_j\rangle = \sum_j c_i \langle A_i \rangle A_j = \sum_j c_i \delta_{ij} = c_i$

2.5 Uncertainty relation between two operators

An interesting application of commutator algebra is to derive a general relation giving the uncertainty product of two Hermitian operators, A and B. Let $\langle A\rangle$ and $\langle B\rangle$ be the expected values of the operators A and B, respectively, with respect to the normalized state vector $|\psi\rangle$. Introducing the operators ΔA and ΔB as:

$$\Delta A = A - \langle A\rangle\,, \qquad \Delta B = B - \langle B\rangle\,, \tag{67}$$

we have $(\Delta A)^2 = A^2 - 2A\langle A\rangle + \langle A\rangle^2$ and $(\Delta B)^2 = B^2 - 2B\langle B\rangle + \langle B\rangle^2$, and hence:

$$\langle \psi \,|\, (\Delta A)^2 \,|\, \psi\rangle = \langle (\Delta A)^2\rangle = \left\langle A^2 - 2A\langle A\rangle + \langle A\rangle^2\right\rangle = \langle A^2\rangle - 2\langle A\rangle\langle A\rangle + \langle A\rangle^2 = \langle A^2\rangle - \langle A\rangle^2 \tag{68}$$

$$\langle \psi \,|\, (\Delta B)^2 \,|\, \psi\rangle = \langle (\Delta B)^2\rangle = \left\langle B^2 - 2B\langle B\rangle + \langle B\rangle^2\right\rangle = \langle B^2\rangle - 2\langle B\rangle\langle B\rangle + \langle B\rangle^2 = \langle B^2\rangle - \langle B\rangle^2 \tag{69}$$

Then, we can write the uncertainties as:

$$\Delta A = \sqrt{\langle (\Delta A)^2\rangle} = \sqrt{\langle A^2\rangle - \langle A\rangle^2}, \qquad \Delta B = \sqrt{\langle (\Delta B)^2\rangle} = \sqrt{\langle B^2\rangle - \langle B\rangle^2} \tag{70}$$

Writing the action of the operators in **Equation 67** on the state vector $|\psi\rangle$, we have:

$$|\chi\rangle = \Delta A\,|\psi\rangle = (A - \langle A\rangle)\,|\psi\rangle\,, \qquad |\phi\rangle = \Delta B\,|\psi\rangle = (B - \langle B\rangle)\,|\psi\rangle \tag{71}$$

The Cauchy-Schwarz inequality[11] gives us:

$$|\langle \chi|\phi\rangle|^2 \le \langle \chi|\chi\rangle\,\langle \phi|\phi\rangle \tag{72}$$

Since A and B are Hermitian, ΔA and ΔB must also be Hermitian, so that: $(\Delta A)^\dagger = \Delta A$ and $(\Delta B)^\dagger = \Delta B$:

$$\langle \chi|\chi\rangle = \left\langle \psi \,\middle|\, (\Delta A)^\dagger(\Delta A) \,\middle|\, \psi\right\rangle = \langle \psi \,|\, (\Delta A)^2 \,|\, \psi\rangle = \langle (\Delta A)^2\rangle \tag{73}$$

$$\langle \phi|\phi\rangle = \left\langle \psi \,\middle|\, (\Delta B)^\dagger(\Delta B) \,\middle|\, \psi\right\rangle = \langle \psi \,|\, (\Delta B)^2 \,|\, \psi\rangle = \langle (\Delta B)^2\rangle \tag{74}$$

$$\langle \chi|\phi\rangle = \left\langle \psi \,\middle|\, (\Delta A)^\dagger(\Delta B) \,\middle|\, \psi\right\rangle = \langle \psi \,|\, \Delta A\Delta B \,|\, \psi\rangle = \langle \Delta A\Delta B\rangle \tag{75}$$

From this, we obtain a new expression for the Cauchy-Schwarz inequality:

$$|\langle \Delta A\Delta B\rangle|^2 \le \langle (\Delta A)^2\rangle\,\langle (\Delta B)^2\rangle \tag{76}$$

We can write the $\Delta A\Delta B$ terms of this equation as:

$$\Delta A\Delta B = 2\cdot\frac{1}{2}\Delta A\Delta B + \frac{1}{2}\Delta B\Delta A - \frac{1}{2}\Delta B\Delta A = \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\} \tag{77}$$

Since $[\Delta A, \Delta B] = [A, B]$[12]:

$$\Delta A\Delta B = \frac{1}{2}[A, B] + \frac{1}{2}\{\Delta A, \Delta B\} \tag{78}$$

Since $[A, B]$ is anti-Hermitian[13] and $[\Delta A, \Delta B]$ is Hermitian[14]; and since the expectation value of a Hermitian operator is real[15] and the expectation value of an anti-Hermitian operator is imaginary[16], $\langle \Delta A\Delta B\rangle$ becomes equal to a real part $\frac{1}{2}\langle\{\Delta A, \Delta B\}\rangle$ plus an imaginary part $\frac{1}{2}\langle [A, B]\rangle$. Then:

$$|\langle \Delta A\Delta B\rangle|^2 = \frac{1}{4}\,|\langle [A, B]\rangle|^2 + \frac{1}{4}\,|\langle \{\Delta A, \Delta B\}\rangle|^2 \ge \frac{1}{4}\,|\langle [A, B]\rangle|^2 \tag{79}$$

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[11] See for more on this inequality in this article.

[12] Check this

[13] *Proof:* As A and B are Hermitian, then $([A, B])^\dagger = (AB - BA)^\dagger = (AB)^\dagger - (BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = BA - AB = -[A, B]$. Then, $[A, B]$ is anti-Hermitian.

[14] *Proof:* As A and B are Hermitian, then $([\Delta A, \Delta B])^\dagger = ((A - \langle A\rangle)(B - \langle B\rangle) - (B - \langle B\rangle)(A - \langle A\rangle))^\dagger = ((A - \langle A\rangle)(B - \langle B\rangle))^\dagger - ((B - \langle B\rangle)(A - \langle A\rangle))^\dagger = (B - \langle B\rangle)^\dagger(A - \langle A\rangle)^\dagger - (A - \langle A\rangle)^\dagger(B - \langle B\rangle)^\dagger = (B - \langle B\rangle)(A - \langle A\rangle) - (A - \langle A\rangle)(B - \langle B\rangle) = [\Delta A, \Delta B]$. Then, $[\Delta A, \Delta B]$ is Hermitian.

[15] See **Section 2.6** for proof.

[16] See **Section 2.7** for proof.

Plugging this into **Equation 76**, we obtain:

$$\frac{1}{4}\left|\langle[A,B]\rangle\right|^2 \leq \left\langle(\Delta A)^2\right\rangle\left\langle(\Delta B)^2\right\rangle \tag{80}$$

Now, taking the square root, we obtain the uncertainty relation:

$$\Delta A \Delta B \geq \frac{1}{2}\left|\langle[A,B]\rangle\right|^2 \tag{81}$$

Definition 2.4. The uncertainty relation between two Hermitian operators A and B is defined as:

$$\Delta A \Delta B \geq \frac{1}{2}\left|\langle[A,B]\rangle\right|^2 \tag{82}$$

2.6 Expected value of a Hermitian operator

From **Equation 22**, we know that the expected value of an operator A in a state $|\phi\rangle$ is $\langle\phi|A|\phi\rangle = \sum_i |c_i|^2\lambda_i$, where c_i are the components of the vector $|\phi\rangle$ in the basis of eigenvectors ψ_i of A, and λ_i are the corresponding eigenvalues. If A is Hermitian ($A^\dagger = A$):

$$\langle A\psi_i|\psi_i\rangle = \lambda^*||\psi_i||^2 \tag{83}$$

$$\langle\psi_i|A^\dagger\psi_i\rangle = \langle\psi_i|A\psi_i\rangle = \lambda||\psi_i||^2 \tag{84}$$

As $\langle A\psi_i|\psi_i\rangle = \langle\psi_i|A^\dagger\psi_i\rangle$, this means that $\lambda^* = \lambda$, so λ must be pure real (or zero). Therefore, the expected value of A must also be pure real.

2.7 Expected value of an anti-Hermitian operator

From **Equation 22**, we know that the expected value of an operator A in a state $|\phi\rangle$ is $\langle\phi|A|\phi\rangle = \sum_i |c_i|^2\lambda_i$, where c_i are the components of the vector $|\phi\rangle$ in the basis of eigenvectors ψ_i of A, and λ_i are the corresponding eigenvalues. If A is anti-Hermitian ($A^\dagger = -A$):

$$\langle A\psi_i|\psi_i\rangle = \lambda^*||\psi_i||^2 \tag{85}$$

$$\langle\psi_i|A^\dagger\psi_i\rangle = -\langle\psi_i|A\psi_i\rangle = -\lambda||\psi_i||^2 \tag{86}$$

As $\langle A\psi_i|\psi_i\rangle = \langle\psi_i|A^\dagger\psi_i\rangle$, this means that $\lambda^* = -\lambda$, so λ must be pure imaginary (or zero). Therefore, the expected value of A must also be pure imaginary.

2.8 Eigenvalues of a Hermitian operator are real and eigenvectors are orthogonal

For a Hermitian operator, all of its eigenvalues are real and the eigenvectors corresponding to different eigenvalues are orthogonal. *Proof:*

Note that:

$$A|\psi_n\rangle = a_n|\psi_n\rangle \rightarrow \langle\psi_m|A|\psi_n\rangle = a_n\langle\psi_m|\psi_n\rangle \tag{87}$$

and:

$$\langle\psi_m|A^\dagger = (A|\psi_m\rangle)^\dagger = (a_m|\psi_m\rangle)^\dagger = a_m^*\langle\psi_m| \rightarrow \langle\psi_m|A^\dagger|\psi_n\rangle = a_m^*\langle\psi_m|\psi_n\rangle \tag{88}$$

Subtracting **Equation 88** from **Equation 87** and using the fact that A is Hermitian ($A^\dagger = A$):

$$\langle\psi_m|A|\psi_n\rangle - \langle\psi_m|A^\dagger|\psi_n\rangle = (a_n - a_m)\langle\psi_m|\psi_n\rangle = (a_n - a_m^*)\langle\psi_m|\psi_n\rangle = 0 \tag{89}$$

From this:

- When $m = n$, we obtain $a_n = a_n^*$, so a_n is real.
- Since, in general, $a_n - a_m^* \neq 0$ when $n \neq m$, we have that $\langle\psi_m|\psi_n\rangle = 0$, so the eigenvectors are orthogonal.

2.9 Common eigenvector basis of two commuting operators

This section gives the proof of **Theorem 1.16**:

Since A has no degenerate eigenvalues[17], to each eigenvalue of A there corresponds only one eigenvector. We can write the eigenvalue equation as:

$$A\,|\phi_n\rangle = a_n\,|\phi_n\rangle \tag{90}$$

And since A commutes with B:

$$AB\,|\phi_n\rangle = BA\,|\phi_n\rangle = Ba_n\,|\phi_n\rangle = a_n B\,|\phi_n\rangle \to A(B\,|\phi_n\rangle) = a_n(B\,|\phi_n\rangle) \tag{91}$$

This means that $B\,|\phi_n\rangle$ is an eigenvector of A with eigenvalue a_n. But since A has no degenerate eigenvalues, $B\,|\phi_n\rangle$ must be proportional to $|\phi_n\rangle$, so that $B\,|\phi_n\rangle = b_n\,|\phi_n\rangle$. Therefore, $|\phi_n\rangle$ is also an eigenvector of B, with eigenvalue b_n.

Since each eigenvector of A is also an eigenvector of B (and vice versa), both of these operators must have a common basis. This basis is unique; it is made of the eigenvectors of A, which are the same as the eigenvectors of B (we say they are joint eigenvectors of A and B). This theorem also holds for any number of mutually commuting Hermitian operators.

[17] Degenerate eigenvalues are those that correspond to more than one eigenvector.