IV. The Abstract Formulation of Quantum Mechanics

4.1. Hilbert Space and Dirac bra-ket Notation

In order to further clarify the underlying mathematical structure of quantum mechanics, consider the properties of the wavefunctions of a system. Since $\rho = |\psi|^2$ is the position probability density we have that ψ must be square-integrable. Further, the principle of superposition implies that $\psi_1+\psi_2$ is a wavefunction if ψ_1 and ψ_2 are wavefunctions. Hence $\psi_1+\psi_2$ is square-integrable as can be seen from

$$|\psi_1+\psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + \underbrace{\psi_1^*\psi_2 + \psi_1\psi_2^*}_{=2\,\mathrm{Re}[\psi_1^*\psi_2]}$$

but $\mathrm{Re}[\psi_1^*\psi_2] \le |\psi_1^*\psi_2| = |\psi_1||\psi_2|$ (i.e. $\mathrm{Re}(z) \le |z|$),

so $$|\psi_1+\psi_2|^2 \le |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2|,$$

further $$(|\psi_1|-|\psi_2|)^2 = |\psi_1|^2+|\psi_2|^2 - 2|\psi_1||\psi_2|$$

implying

$$|\psi_1+\psi_2|^2 \le 2|\psi_1|^2 + 2|\psi_2|^2 - (|\psi_1|-|\psi_2|)^2$$
$$\le 2|\psi_1|^2 + 2|\psi_2|^2 .$$

If ψ_1, ψ_2 are square-integrable

$$\int d^3r\, |\psi_1|^2 < \infty$$

$$\int d^3r\, |\psi_2|^2 < \infty \quad \text{, then}$$

$$\int d^3r\, |\psi_1 + \psi_2|^2 \leq 2\int d^3r\, |\psi_1|^2 + 2\int d^3r\, |\psi_2|^2$$

$< \infty$, so $\psi_1 + \psi_2$ is also

square-integrable. Thus we are led to consider the vector space formed by the square integrable wavefunctions. It is called $L^2(\mathbb{R}^3)$ and is a Hilbert space. A Hilbert space is an example of a complex vector space.

(In practice we add other restrictions to ψ than just square-integrability. For instance we can consider continuous functions or differentiable functions or C_∞ functions for that matter. Since sums of C_∞ functions are still C_∞, etc., we are considering subspaces of $L^2(\mathbb{R}^3)$ functions, that is subspaces of the Hilbert space. Since we can approximate any function of L^2 by a sum of smooth

C^∞ functions we observe that the limit points of sequences of functions in our subspace of functions, call it $C(\mathbb{R}^3)$, may not be elements of $C(\mathbb{R}^3)$. It is said that $C(\mathbb{R}^3)$ is not complete (like an open interval). If we add to C its "limit points" we close or complete the space (like a closed interval), we denote the closure of C as $\overline{C}(\mathbb{R}^3)$. It can be shown that $\overline{C}(\mathbb{R}^3) = L^2(\mathbb{R}^3)$. The possible wavefunctions of a quantum mechanical system will be functions of L^2. They form a vector space which is closed. This is known as a Hilbert space. The point of all this being we only observe a wavefunction's continuity on scales the order of 10^{-16} cm, thus we can always approximate the discontinuous function with a sum of continuous ones. We really only deal with functions in $C(\mathbb{R}^3)$. But in principle all $L^2(\mathbb{R}^3)$ functions can represent a state of the system.) (by principle of superposition

Recall that a complex vector space V is a set of elements (vectors) ψ, ϕ, etc., such that $\psi+\phi$ is also a vector when ψ and ϕ are vectors and $\lambda\psi$ is a vector if ψ is a vector and $\lambda \in \mathbb{C}$. As well the vector addition and multiplication of a vector by a complex number obey

$$\psi + \phi = \phi + \psi$$

$$\psi + (\phi + \chi) = (\psi + \phi) + \chi$$

$$\lambda(\phi + \psi) = \lambda\phi + \lambda\psi$$

$$(\lambda + \omega)\phi = \lambda\phi + \omega\phi$$

$$\lambda(\omega\phi) = (\lambda\omega)\phi$$

where ψ, ϕ, χ are vectors and $\lambda, \omega \in \mathbb{C}$. In addition there exists a unique vector $\underline{O}$ for which

$$\underline{O} + \psi = \psi$$

vector zero $\underline{O}$

$$0\psi = \underline{O}$$

vector zero $\underline{O}$

number zero

Examples: 1) L^2 (or restrictions to smooth functions S) is a complex vector space since the sum of wavefunctions and their product with a complex number is again a wavefunction in L^2 (principle of superposition)

2) The set of all n-tuples of complex numbers

$(z_1, z_2, \ldots, z_n)$ (n may be ∞) with addition defined by

$$(w_1, w_2, \ldots, w_n) + (z_1, z_2, \ldots, z_n) = (w_1+z_1, w_2+z_2, \ldots, w_n+z_n)$$

and multiplication of a vector by $\lambda \in \mathbb{C}$ defined by

$$\lambda(z_1, z_2, \ldots, z_n) = (\lambda z_1, \lambda z_2, \ldots, \lambda z_n) .$$

In addition to the above properties which define a complex vector space, such a space may also allow a <u>scalar product</u> or <u>inner product</u>, denoted (ϕ, ψ), to be defined on it with the properties that $(\phi, \psi) \in \mathbb{C}$ and

$$(\psi,\phi)^* = (\phi,\psi)$$

$$(\phi,\psi_1+\psi_2) = (\phi,\psi_1) + (\phi,\psi_2)$$

$$(\phi,\lambda\psi) = \lambda(\phi,\psi) \qquad (\Rightarrow (\phi,\underline{0})=0)$$

$$(\psi,\psi) > 0 \text{ except for } \psi=\underline{0}$$
when $(\underline{0},\underline{0})=0$.

Note that the scalar product is <u>linear</u> in the second entry

$$(\phi,\psi_1+\lambda\psi_2) = (\phi,\psi_1)+\lambda(\phi,\psi_2),$$

but <u>anti-linear</u> in the first entry

$$(\phi_1+\lambda\phi_2,\psi) = (\phi_1,\psi) + \lambda^*(\phi_2,\psi).$$

Also the inner product obeys the Schwarz inequality

$$|(\psi_1,\psi_2)|^2 \le (\psi_1,\psi_1)(\psi_2,\psi_2).$$

<u>Proof</u>: Consider the vector

$$\psi = \psi_1 + \lambda\psi_2 \text{ with } \lambda\in\mathbb{C} \text{ an}$$
arbitrary complex number

Then by the definition of the inner product
$(\psi,\psi) \geq 0 \Rightarrow$

$$F(\lambda,\lambda^*) \equiv (\psi,\psi) = (\psi_1,\psi_1) + \lambda(\psi_1,\psi_2) + \lambda^*(\psi_2,\psi_1) + \lambda^*\lambda(\psi_2,\psi_2) \geq 0$$

$F(\lambda,\lambda^*)$ can be minimized by looking at the λ-derivative

$$\left.\frac{dF}{d\lambda}\right|_{\substack{\lambda=\lambda_{min}\\ \lambda^*=\lambda^*_{min}}} = 0 = (\psi_1,\psi_2) + \lambda^*_{min}(\psi_2,\psi_2)$$

$$\left.\frac{dF}{d\lambda^*}\right|_{\substack{\lambda^*=\lambda^*_{min}\\ \lambda=\lambda_{min}}} = 0 = (\psi_2,\psi_1) + \lambda_{min}(\psi_2,\psi_2)$$

$$\Rightarrow \qquad \lambda_{min} = -\frac{(\psi_2,\psi_1)}{(\psi_2,\psi_2)}$$

and as required

$$\lambda^*_{min} = -\frac{(\psi_1,\psi_2)}{(\psi_2,\psi_2)} = -\frac{(\psi_2,\psi_1)^*}{(\psi_2,\psi_2)}$$

Since $(\psi,\psi)^* = (\psi,\psi)$ is real.

Substituting above $F(\lambda_{min},\lambda^*_{min}) \geq 0$ yields the Schwarz inequality.

The equality sign holds iff $(\psi,\psi)=0$, that is

$\psi_1 = -\lambda\psi_2$, that is ψ_1 and ψ_2 are multiples of each other ("parallel").

Using the inner product a <u>norm</u> of a vector can be defined as

$$\|\psi\| \equiv (\psi,\psi)^{\frac{1}{2}}$$

which is real and positive, $\|\psi\|>0$, unless $\psi=\underline{0}$ then $\|\underline{0}\|=0$.

<u>Examples</u> i) The scalar product in $L^2(\mathbb{R}^3)$ (or $S(\mathbb{R}^3)$) is defined by the space-integral of the product of wavefunctions, for $\psi(\vec{r})$ and $\phi(\vec{r}) \in L^2(\mathbb{R}^3)$ we have

$$(\phi,\psi) \equiv \int d^3r\, \phi^*(\vec{r})\psi(\vec{r}),$$ the

required properties of the inner product can be checked directly. The norm squared of a vector is just seen to be the usual quantum mechanical normalization of the wavefunction

$$\|\psi\|^2 = (\psi,\psi) = \int d^3r\, \psi^*(\vec{r})\psi(\vec{r}).$$

2) The space of all n-tuples of complex numbers $(z_1, z_2, \ldots, z_n)$ with

$$\sum_{i=1}^{n} |z_i|^2 < \infty \qquad (n \text{ may be } \infty).$$

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The inner product is given by

$$(w, z) \equiv \sum_{i=1}^{n} w_i^* z_i$$

where $z = (z_1, \ldots, z_n)$; $w = (w_1, \ldots, w_n)$.

Note that this sum is finite even in the case that n is infinite since

$$\left| \sum_{i=1}^{n} w_i^* z_i \right| \leq \sum_{i=1}^{n} |w_i||z_i|$$

$$= \frac{1}{2} \sum_{i=1}^{n} \left(|w_i|^2 + |z_i|^2 - (|w_i| - |z_i|)^2 \right)$$

$$\leq \frac{1}{2} \sum_{i=1}^{n} \left(|w_i|^2 + |z_i|^2 \right) < \infty$$

since $\sum_{i=1}^{n} |z_i|^2 < \infty$ and $\sum_{i=1}^{n} |w_i|^2 < \infty$.

Further, all the properties of the inner product are obeyed as can be checked directly. The norm of a

That this set is a vector space follows from the fact that the sum of two n-tuples is also an n-tuple that obeys the finite norm sum, that is if $\sum_{i=1}^{n_f} |z_i|^2 < \infty$ and $\sum_{i=1}^{n_f} |w_i|^2 < \infty$ then

$$\sum_{i=1}^{n_f} |z_i + w_i|^2 = \sum_{i=1}^{n_f} \left(|z_i|^2 + |w_i|^2 + 2\,\mathrm{Re}(z_i^* w_i) \right)$$

(Since $\mathrm{Re}\, z \le |z|$)

$$\le \sum_{i=1}^{n_f} \left(|z_i|^2 + |w_i|^2 + 2|z_i||w_i| \right)$$

$$\le \sum_{i=1}^{n_f} \left(|z_i| + |w_i| \right)^2$$

$$\le \sum_{i=1}^{n_f} \left[2|z_i|^2 + 2|w_i|^2 - \left(|z_i| - |w_i| \right)^2 \right]$$

$$\le 2 \sum_{i=1}^{n_f} \left(|z_i|^2 + |w_i|^2 \right) < \infty .$$

vector is given by

$$\|z\| = (z,z)^{1/2} = \sqrt{\sum_{i=1}^{n} |z_i|^2} > 0$$

unless $z_i = 0$ for each i, that is unless $z = \underline{0}$; then $\|z\| = \|\underline{0}\| = 0$.

The norm of a sum of 2 vectors is given by

$$\|w+z\|^2 = \sum_{i=1}^{n} |w_i + z_i|^2$$

$$= \sum_{i=1}^{n} \Big(|w_i|^2 + |z_i|^2 + w_i^* z_i + z_i^* w_i \Big)$$

$$= \|w\|^2 + \|z\|^2 + \underbrace{(w,z) + (z,w)}_{=2\mathrm{Re}(w,z)}$$

$$\leq \|w\|^2 + \|z\|^2 + 2|(w,z)|$$

but the Schwarz inequality yields

$$|(w,z)| \leq (w,w)^{1/2} (z,z)^{1/2}$$

$$\leq \|w\| \, \|z\|$$

So

$$\|w+z\|^2 \leq \|w\|^2 + \|z\|^2 + 2\|w\|\|z\|$$

$$\leq \big(\|w\| + \|z\|\big)^2$$

Hence

$$\|w+z\| \leq \|w\| + \|z\|$$, this is known as the triangle inequality. The norm of a sum of 2 vectors is less than or equal to the sum of the norms of the vectors.

Notice it can be shown that equality holds only if $w=0$ or $w=\lambda z$ with $\lambda \geq 0$.

From the above discussion, it is clear that the triangle inequality holds for abstract inner product complex vector spaces also

$$\|\psi+\phi\|^2 = (\psi+\phi, \psi+\phi)$$

$$= (\psi,\psi) + (\phi,\phi) + (\psi,\phi) + (\phi,\psi)$$

$$= \|\psi\|^2 + \|\phi\|^2 + 2\,\mathrm{Re}\left[(\psi,\phi)\right]$$

$$\leq \|\psi\|^2 + \|\phi\|^2 + 2\,|(\psi,\phi)|$$

by the Schwarz inequality

$$|(\psi,\phi)| \leq \|\psi\|\,\|\phi\|$$

So

$$\|\psi+\phi\|^2 \leq \|\psi\|^2 + \|\phi\|^2 + 2\|\psi\|\,\|\phi\|$$

$$\leq \left(\|\psi\| + \|\phi\|\right)^2$$

So
$$\|\psi+\phi\| \le \|\psi\| + \|\phi\|$$ with

equality holding only if
$$(\psi,\phi) = \|\psi\|\,\|\phi\|$$

but if $\psi \neq 0$ this is true only if

$\psi = \lambda\phi$ by the Schwarz inequality, hence
$$(\psi,\phi) = (\lambda\phi,\phi) = \lambda^*(\phi,\phi) = \|\lambda\phi\|\,\|\phi\|$$

$$\Rightarrow \quad \lambda^*(\phi,\phi) = |\lambda|\,(\phi,\phi)$$

hence λ is real and positive. So we obtain the triangle inequality

$$\|\psi+\phi\| \le \|\psi\| + \|\phi\|$$

with equality only if $\psi=0$ or $\psi=\lambda\phi$ and $\lambda \ge 0$.

The inner product space, that is a complex vector space with an inner product, is a <u>metric space</u> with the distance between two vectors given in terms of the norm

$\|\psi - \phi\| \equiv d(\psi,\phi)$ the distance between ψ and ϕ. This definition of distance obeys the usual properties of a distance function

$$d(\psi,\phi) = d(\phi,\psi) > 0 \quad \text{for } \psi \neq \phi$$

$$d(\psi,\psi) = 0$$

$$d(\psi,\phi) \leq d(\psi,\chi) + d(\chi,\phi)$$

(triangle inequality).

The distance or metric allows a concept of closeness (topology) to be introduced into the space, that is neighborhoods of a vector. Further, a sequence of vectors ψ_n has a limit point ψ in the space if

$$\lim_{n\to\infty} d(\psi,\psi_n) = 0$$

That is $\psi_n \to \psi$ or $\lim_{n\to\infty} \psi_n = \psi$ if

$$\lim_{n\to\infty} \|\psi - \psi_n\| = 0.$$

In fact using the triangle inequality

$$\lim_{m,n\to\infty} \|\psi_m - \psi_n\| \leq \|\psi_m - \psi\| + \|\psi - \psi_n\| = 0$$

where m and n independently go to ∞.

Such a sequence $\lim_{\substack{m\to\infty \\ n\to\infty}} \|\psi_m - \psi_n\| = 0$

is call a Cauchy sequence.

It could happen that not every sequence of vectors in the space converges to an element of the space.

A metric space is called complete if every Cauchy sequence in the space converges to some element of the space.

A complex vector space with an inner product which is complete in the norm induced by the inner product is called a Hilbert space, denoted $\mathcal{H}$.

Thus every Cauchy sequence of vectors in $\mathcal{H}$ $\{\psi_1, \psi_2, \psi_3, \ldots\}$ with

$$\lim_{\substack{m\to\infty \\ n\to\infty}} \|\psi_m - \psi_n\| = 0,$$

converges to a vector $\psi \in \mathcal{H}$, $\lim_{n\to\infty} \psi_n = \psi$

that is

$$\lim_{n\to\infty} \|\psi - \psi_n\| = 0 \quad , \text{with } \psi \in \mathcal{H}.$$

examples: 1) The space of square-integrable functions $L^2(\mathbb{R}^3)$ with the previously defined inner product; $\psi(\vec{r}), \phi(\vec{r}) \in L^2$

$$(\psi, \phi) \equiv \int d^3r \, \psi^*(\vec{r}) \phi(\vec{r}) \, .$$

(This space is infinite dimensional)

Hence a Cauchy sequence of wavefunctions $(\psi_1, \psi_2, \ldots)$ obeys the limit

$$\lim_{\substack{m\to\infty \\ n\to\infty}} \int d^3r \, |\psi_m(\vec{r}) - \psi_n(\vec{r})| = 0$$

It is left to the student to show that $L^2(\mathbb{R}^3)$ is complete and hence a Hilbert space, that's every Cauchy sequence of L^2 functions converges to an L^2 function

$$\lim_{n\to\infty} \int d^3r \, |\psi(\vec{r}) - \psi_n(\vec{r})| = 0$$

where $\int d^3r \, |\psi(\vec{r})|^2 < \infty$.

2) The space of all finite norm n-tuples of complex numbers, $(z_1, \ldots, z_n) = z$ with

$$(z, z) = \|z\|^2 = \sum_{i=1}^{n} |z_i|^2 < \infty,$$ is a Hilbert space.

Clearly all finite dimensional inner product spaces have only finite sequences and hence are Hilbert spaces. For $n = \infty$, this space of n-tuples is also complete in the norm. Each Cauchy sequence of ∞-tuples $(z^{(1)}, z^{(2)}, \ldots)$

$$\lim_{m,n\to\infty} \|z^{(m)} - z^{(n)}\| = \left(\sum_{i=1}^{\infty} |z_i^{(m)} - z_i^{(n)}|^2\right)^{1/2} = 0$$

converges to ~~an~~ a finite norm ∞-tuple of complex numbers

$$\lim_{n\to\infty} \|z - z^{(n)}\| = \left(\sum_{i=1}^{\infty} |z_i - z_i^{(n)}|^2\right)^{1/2} = 0$$

and $\|z\|^2 = \sum_{i=1}^{\infty} |z_i|^2 < \infty$. This just follows from the completeness of the complex (real) numbers. So indeed the space of finite norm n-tuples of complex numbers is a Hilbert space for finite or infinite.

Thus the underlying mathematical structure of quantum mechanics begins to emerge. The wavefunctions $\psi(\vec{r})$ are in correspondence with the vectors of a Hilbert space. As we know instead of the position probability amplitude $\psi(\vec{r})$ to describe a system we could determine all physical quantities from the momentum probability amplitude $g(\vec{k}) = \int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\, \psi(\vec{r})$.

These momentum space wavefunctions are square-integrable since they correspond to a probability density and have an inner product given by

$$(g, f) \equiv \int \frac{d^3k}{(2\pi)^3}\, g^*(\vec{k}) f(\vec{k}) \, ,$$

they are just $L^2(\mathbb{R}^3)$ functions again with finite norm. The momentum space wavefunctions also lie in correspondence with vectors in the same Hilbert space and are equally good to describe the states of the system as are the position space wavefunctions $\psi(\vec{r})$.

Well this is all reminiscent of

the case in Euclidean 3-space ($E^3 = R^3$) where a vector $\vec{v}$ can be equally well described by its coordinates with respect to different bases. Each component representation of the vector being a completely equivalent description of the abstract geometric vector.

Similarly we see that the state of a system is described by an abstract vector in Hilbert space $\mathcal{H}$. Each description of the vector in terms of different bases, like the position space components given by the wavefunctions $\psi(\vec{r})$ or the momentum space components given by the momentum wavefunctions $g(\vec{k})$ is an equivalent representation of the underlying vectors in the Hilbert space.

Just as the 3-vector $\vec{v}$ can be expanded in terms of different bases vectors

$$\vec{v} = \sum_{i=1}^{3} v_i \, \hat{e}^{(i)} = \sum_{i=1}^{3} v_i' \, \hat{e}'^{(i)}$$

where v_i are the components of $\vec{v}$ in the $\hat{e}^{(i)}$-system and v_i' are the components of $\vec{v}$ in the $\hat{e}'^{(i)}$-system, So too we can view the $\psi(\vec{r})$ and $g(\vec{k})$ as the components of the coordinate free abstract vector ψ in 2 different bases, the coordinate and momentum bases. And just as the 3-vector components v_i and v_i' can be given in terms of the inner product of the basis vectors and $\vec{v}$

$$v_i = \hat{e}^{(i)} \cdot \vec{v} \quad ; \quad v_i' = \hat{e}'^{(i)} \cdot \vec{v},$$

So too we can represent the spatial and momentum wavefunctions, as we shall see.

To make clear these observations it is useful to introduce a notation for vectors and inner product that was developed by Dirac called Dirac (bra-ket) notation.

Instead of just calling each vector in the Hilbert space by ψ, ϕ, etc. Dirac enclosed them in a ket notation and the vectors are called ket-vectors, so we have that

$|\psi\rangle$, $|\phi\rangle$, etc. denote the vectors in our Hilbert space.

The label inside $| \rangle$ denotes the element of the space under consideration. So in this Dirac notation we write the sum of two vectors as $|\psi\rangle + |\phi\rangle$, and the multiplication of a vector by a complex number λ as $\lambda|\psi\rangle$. The ket vector for $\lambda\psi$ is just this product, $|\lambda\psi\rangle \equiv \lambda|\psi\rangle$ in Dirac notation.

Given any vector space we can always define another vector space dual to it by considering the set of all linear functionals (maps) on the space. A linear functional ϕ is a map of $\mathcal{H}$ into the complex numbers that is linear, for $|\chi\rangle, |\psi\rangle \in \mathcal{H}$

$$\phi(|\psi\rangle) \in \mathbb{C} \quad \text{and}$$

$$\phi(|\psi\rangle + \lambda|\chi\rangle) = \phi(|\psi\rangle) + \lambda\phi(|\chi\rangle).$$

Further a bounded linear functional is a linear functional for which

$$|\phi(|\psi\rangle)| \leq M \, \| |\psi\rangle \| \quad , \quad M < \infty,$$

where recall $\| |\psi\rangle \| = (|\psi\rangle, |\psi\rangle)^{1/2}$.

The norm of ϕ is defined as the minimum value of M for all $|\psi\rangle$ in $\mathcal{H}$

$$\|\phi\| \equiv M_\phi = \inf\{M \geq 0 : |\phi(|\psi\rangle)| \leq M \, \| |\psi\rangle \| \text{ for } \forall |\psi\rangle \in \mathcal{H}\}.$$

The set of all linear functionals on $\mathcal{H}$ defines a vector space called the <u>dual (space) to $\mathcal{H}$</u> and is denoted $\mathcal{H}^*$. That is if ϕ and Ω are linear functionals then

$$(\phi+\Omega)(|\psi\rangle) \equiv \phi(|\psi\rangle) \underset{\substack{\uparrow \\ \text{addition of} \\ \text{complex numbers}}}{+} \Omega(|\psi\rangle)$$

and $\lambda\phi(|\psi\rangle)$ are again linear functionals. (The set of all bounded linear functionals in fact form a normed vector space with norm defined by $\|\phi\| = M_\phi$.) Further the addition of functionals and their multiplication by complex numbers obey all the required properties of a vector space.

According to the notation of Dirac, the vectors in $\mathcal{H}^*$ are denoted by a <u>bra</u> notation $\langle\phi|$ and are called <u>bras</u> or <u>bra vectors</u>. The label inside $\langle\ |$ denotes the vector of $\mathcal{H}^*$ under consideration.

Dirac then uses a bra-ket (bracket) notation to represent the mapping of each linear functional $\phi(|\psi\rangle)$. That is he writes $\phi(|\psi\rangle)$ as

$$\phi(|\psi\rangle) = \langle\phi|\psi\rangle.$$

The inner product in $\mathcal{H}$ defines a bounded linear functional. For $|\phi\rangle \in \mathcal{H}$

$$\left(\phi(|\psi\rangle) =\right) \langle\phi|\psi\rangle \equiv (|\phi\rangle, |\psi\rangle) \text{ is}$$

a linear functional with norm $\| \langle\phi| \| = \| |\phi\rangle \|$.

Thus for every ket in $\mathcal{H}$, $|\phi\rangle \in \mathcal{H}$, their corresponds a bra in $\mathcal{H}^*$, $\langle\phi| \in \mathcal{H}^*$ defined by the inner product

$$\langle\phi|\psi\rangle = (|\phi\rangle, |\psi\rangle).$$

Since we have just shown that to every ket vector there corresponds a bra vector, we can ask whether there is a ket vector corresponding to every bra-vector. A theorem due to Riesz guarantees the correspondence for bounded linear functionals

Riesz's Theorem: Every bounded linear functional $(\phi =)\ \langle\phi|$ can be expressed in the form

$$(\phi(|\psi\rangle) =)\ \langle\phi|\psi\rangle = (|\phi\rangle, |\psi\rangle)$$

where $|\phi\rangle$ is an element of $\mathcal{H}$ uniquely determined by $\langle\phi|$ and $(|\phi\rangle, |\psi\rangle)$ is the inner product in $\mathcal{H}$.

For a proof see

1) Akhiezer and Glazman: "Theory of Linear Operators in Hilbert Space Vol. 1." page 33.
2) Riesz and Sz.-Nagy: "Functional Analysis" page 61.
3) Stakgold: "Boundary Value Problems of Mathematical Physics Vol 1" page 136.

4) Jauch: "Foundations of Quantum Mechanics", page 31.

The idea of the proof is simply to expand any vector $|\psi\rangle$ in terms of any orthonormal basis of vectors $|e_n\rangle$

$$|\psi\rangle = \sum_n{}' c_n |e_n\rangle$$

Then any functional $\langle\phi|$ can be written as

$$\langle\phi|\psi\rangle = \sum_n{}' c_n \langle\phi|e_n\rangle .$$

The ket vector in $\mathcal{H}$, $|\phi\rangle$, corresponding to the $\langle\phi|$ is

$$|\phi\rangle \equiv \sum_n{}' \langle\phi|e_n\rangle^* |e_n\rangle$$

Since

$$(|\phi\rangle, |\psi\rangle) = \sum_{m,n}{}' (\langle\phi|e_n\rangle^* |e_n\rangle, c_m |e_m\rangle)$$

$$= \sum_{m,n}{}' \langle\phi|e_n\rangle c_m \underbrace{(|e_n\rangle, |e_m\rangle)}_{=\delta_{mn}}$$

$$= \sum_n{}' c_n \langle\phi|e_n\rangle$$

$$= \langle\phi|\psi\rangle .$$

Thus $\mathcal{H}$ and $\mathcal{H}^*$ are isomorphic.

In fact using Riesz's Theorem one can define a scalar product in $\mathcal{H}^*$, it is just that of corresponding kets in $\mathcal{H}$, and show that $\mathcal{H}^*$ is a Hilbert Space.

Since every functional has the form

$$\langle \phi | \psi \rangle = (|\phi\rangle, |\psi\rangle)$$

we will use the Dirac bra-ket notation to denote the inner product from now on. Recalling the properties of the inner product using Dirac notation (e.g. page-244)

1) $\langle \psi | \phi \rangle^* = \langle \phi | \psi \rangle$

2) $\langle \phi | \psi_1 + \psi_2 \rangle = \langle \phi | \psi_1 \rangle + \langle \phi | \psi_2 \rangle$

3) $\langle \phi | \lambda \psi \rangle = \lambda \langle \phi | \psi \rangle$

4) $\langle \psi | \psi \rangle \geq 0$ with equality only if $|\psi\rangle = 0$.

Properties 2) & 4) express the linearity of the functional in the ket-vector

$$\langle\phi|\psi_1+\lambda\psi_2\rangle = \langle\phi|\psi_1\rangle + \lambda\langle\phi|\psi_2\rangle$$

Property 1) implies as previously the functional is anti-linear in the bra-vector

$$\langle\phi_1+\lambda\phi_2|\psi\rangle = \langle\phi_1|\psi\rangle + \lambda^*\langle\phi_2|\psi\rangle.$$

The inner product associates the bra-vector $\langle\phi_1| + \lambda^*\langle\phi_2|$ in $\mathcal{H}^*$ with the ket-vector $|\phi_1\rangle + \lambda|\phi_2\rangle$ in $\mathcal{H}$. (i.e. the bra corresponding to $|\lambda\phi\rangle = \lambda|\phi\rangle$ is $\langle\lambda\phi| = \lambda^*\langle\phi|$. The bra-vectors are like the complex conjugate of the wave functions, to each $\psi(\vec{r})$ there corresponds a $\psi^*(\vec{r})$ and vice versa. Corresponding to $\lambda\psi(\vec{r})$ is $(\lambda\psi(\vec{r}))^* = \lambda^*\psi^*(\vec{r})$.)

(Technical Aside: as we have seen, it is useful to introduce non-normalizable vectors, hence not belonging to ($\mathcal{H}$) L^2, in terms of which we may expand the normalizable vectors.) For example plane-waves in 1-dimension are non-normalizable basis vectors

$$\psi(x) = \int_{-\infty}^{+\infty} \frac{dp}{(2\pi\hbar)}\, e^{\frac{i}{\hbar}px}\, \tilde{\psi}(p)$$

$$\tilde{\psi}(p) = \int_{-\infty}^{+\infty} dx\, e^{-\frac{i}{\hbar}px}\, \psi(x) .$$

This can be interpreted as expanding our state vectors ψ in terms of basic vectors $\{u_p(x)\}$ with p a continuous index labelling their components i.e.

$$u_p(x) \equiv e^{\frac{i}{\hbar}px} .$$

As we know these basis vectors are complete

$$\int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar}\, u_p^*(y)\, u_p(x) = \delta(x-y)$$

and are "normalized" according to "Continuum normalization conditions"

$$\int_{-\infty}^{+\infty} dx\, u_p^*(x)\, u_{p'}(x) = \delta(p-p') .$$

The abstract vector corresponding to the plane-wave function $u_p(x)$ we denote

$$|u_p\rangle ,$$

it is not an element of the Hilbert space of physical vectors $|u_p\rangle \notin \mathcal{H}$.

However

$$\langle u_p|\psi\rangle = \int_{-\infty}^{+\infty} dx\, u_p^*(x)\, \psi(x)$$

$$= \tilde{\psi}(p) \in \mathbb{C} .$$

The Fourier transform defines a linear functional, thus $\langle u_p|$ is an element of the dual space of linear functionals but $|u_p\rangle \notin \mathcal{H}$. In order to maintain the symmetry of states in $\mathcal{H}$ and the dual space to $\mathcal{H}$, we extend our Hilbert space $\mathcal{H}$ to include generalized kets with infinite (continuum) norms but whose scalar product with every ket of $\mathcal{H}$ is finite. This extended space is denoted $\hat{\mathcal{H}}$ and is isomorphic to the extension of the space of bounded linear functionals $\mathcal{H}^*$. (Thus to each bra vector $\langle \psi |$ of $\hat{\mathcal{H}}^*$ there corresponds a ket-vector $|\psi\rangle \in \hat{\mathcal{H}}$ and vice-versa.)

From now on we will use Dirac notation when considering vector spaces.

In particular two vectors $|\psi\rangle$ and $|\phi\rangle$ are said to be orthogonal if

$$\langle \phi | \psi \rangle = 0.$$

A set of vectors $|\psi_1\rangle, |\psi_2\rangle, \ldots$ is independent if there is no set of complex numbers $\lambda_1, \lambda_2, \ldots$ for which the equation

$$\lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle + \cdots = 0$$

is satisfied <u>except</u> $\lambda_1 = \lambda_2 = \cdots = 0$.

Note, any set of orthogonal vectors $\{|\psi_k\rangle\}$ is independent since

$$0 = \sum_k{}' \lambda_k |\psi_k\rangle$$

$$\Rightarrow \quad 0 = \langle \psi_j | \sum_k{}' \lambda_k \psi_k \rangle = \sum_k{}' \lambda_k \overbrace{\langle \psi_j | \psi_k \rangle}^{=\langle \psi_j | \psi_j \rangle \delta_{jk}}$$

$$= \lambda_j \langle \psi_j | \psi_j \rangle$$

$$\Rightarrow \lambda_j = 0 .$$

A vector space has <u>dimensionality</u> N if the maximum number of independent vectors is N. Any set of N-independent vectors $\{|\psi_k\rangle\}$ in such a space is <u>complete</u>, because given any vector $|\psi\rangle$, there must be some (unique), non-trivial linear relation

$$0 = \lambda|\psi\rangle + \sum_k^{\prime} \lambda_k |\psi_k\rangle$$

with $\lambda \neq 0$ (otherwise the dimension is $(N+1)$)

For a N-dimensional space, no set of $M<N$ vectors is complete.

<u>Proof</u>: Let $\{|\psi_k\rangle\}$ be a complete independent set of M vectors, and let $\{|\phi_k\rangle\}$ be a complete independent set of N vectors.

Then 1) $|\phi_1\rangle$ must be a linear combination of $|\psi_1\rangle, \cdots, |\psi_M\rangle$

2) Let $|\psi_k\rangle$ be any vector in this linear combination

Then
$$|\psi_1\rangle, \ldots, |\psi_{k-1}\rangle, |\phi_1\rangle, |\psi_{k+1}\rangle, \ldots, |\psi_M\rangle$$
must be a complete independent set,

3) Repeat this process with $|\phi_2\rangle$, then
$$|\psi_1\rangle, \ldots, |\psi_{k-1}\rangle, |\phi_1\rangle, |\psi_{k+1}\rangle, \ldots, |\psi_{\ell-1}\rangle, |\phi_2\rangle,$$
$$|\psi_{\ell+1}\rangle, \ldots, |\psi_M\rangle$$
is a complete independent set.

4) Continue this procedure until all the $|\psi_k\rangle$ vectors are eliminated.

But then $|\phi_1\rangle, \ldots, |\phi_M\rangle$ is a complete set. Hence $|\phi_1\rangle, \ldots, |\phi_N\rangle$ cannot be independent for $N > M$, this is a contradiction.

Infinite dimensionality means that there is no maximum number of independent vectors. The above theorem shows that no finite set of vectors can be complete in an infinite-dimensional space.

Discrete Orthonormal Basis in $\mathcal{H}$: If $\{|\phi_k\rangle\}$ forms a complete independent set of vectors, then any arbitrary ket vector $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \sum_k{}' c_k |\phi_k\rangle .$$

The $\{c_k\}$ are the components of $|\psi\rangle$ in the $\{|\phi_k\rangle\}$ basis. The uniqueness of $\{c_k\}$ follows from the independence of $\{|\phi_k\rangle\}$.

Moreover, if the $\{|\phi_k\rangle\}$ basis is an orthonormal basis, that is $\langle\phi_k|\phi_\ell\rangle = \delta_{k\ell}$

then $\langle\phi_\ell|\psi\rangle = \langle\phi_\ell|\sum_k' c_k\phi_k\rangle$

$$= \sum_k' c_k\langle\phi_\ell|\phi_k\rangle = \sum_k' c_k\delta_{\ell k}$$
$$= c_\ell \quad .$$

Hence for any $|\psi\rangle$

$$|\psi\rangle = \sum_k' c_k|\phi_k\rangle$$
$$= \sum_k' |\phi_k\rangle\langle\phi_k|\psi\rangle$$

Since $|\psi\rangle$ is arbitrary, we have

$$\sum_k' |\phi_k\rangle\langle\phi_k| = 1 \ , \quad \left(\begin{array}{c}1 \text{ is the} \\ \text{identity operator} \\ \text{in } \mathcal{H}\end{array}\right)$$

The operator $|\phi_k\rangle\langle\phi_k| \equiv P_k$ is the projection operator on to the $|\phi_k\rangle$ vector. $\sum_k' |\phi_k\rangle\langle\phi_k| = 1$ is the completeness or closure identity for the basis vectors $\{|\phi_k\rangle\}$.

Further if $|\psi\rangle = \sum_k' c_k|\phi_k\rangle$ and

$|\psi'\rangle = \sum_k' c_k'|\phi_k\rangle$ then

$\langle\psi'| = \langle \sum_k^f c_k' \phi_k| = \sum_k^f c_k'^* \langle\phi_k|$, recall

due to the anti-linearity of the inner product bra and ket vectors are anti-linearly related, they are conjugates of each other,

So $\langle\psi'|\psi\rangle = \langle \sum_k^f c_k'\phi_k | \sum_l^f c_l \phi_l\rangle$

$$= \sum_k^f \sum_l^f c_k'^* c_l \langle\phi_k|\phi_l\rangle$$

$$= \sum_k^f c_k'^* c_k$$

and the norm of $|\psi\rangle$, is given by $\|\psi\|^2 = \langle\psi|\psi\rangle = \sum_k^f |c_k|^2$.

If $\{|\phi_k\rangle\}$ forms an independent set,

then $|\psi_1\rangle = \lambda_{11}|\phi_1\rangle$

$$|\psi_2\rangle = \lambda_{21}|\phi_1\rangle + \lambda_{22}|\phi_2\rangle$$

$$|\psi_3\rangle = \lambda_{31}|\phi_1\rangle + \lambda_{32}|\phi_2\rangle + \lambda_{33}|\phi_3\rangle$$

$\vdots$

can be chosen as an orthonormal set, by the Gramm-Schmidt Process.

Proof: This is true for 1 vector by letting

$$\lambda_{11} = \frac{1}{\sqrt{\langle \phi_1 | \phi_1 \rangle}}.$$

Assume it is true for n vectors, then choose

$$|\psi_{n+1}\rangle = C\left[\rho_1|\psi_1\rangle + \cdots + \rho_n|\psi_n\rangle + |\phi_{n+1}\rangle\right]$$

where $C = \lambda_{(n+1)(n+1)}$ and for $0 \le k \le n$

$$0 = \langle \psi_k, \psi_{n+1}\rangle = C\rho_k + C\langle \psi_k | \phi_{n+1}\rangle.$$

Hence $\boxed{\rho_k = -\langle \psi_k | \phi_{n+1}\rangle}$. In addition

$$\begin{aligned} 1 &= \langle \psi_{n+1} | \psi_{n+1}\rangle \\ &= |C|^2\Big\{\sum_{k=1}^{n} |\rho_k|^2 + \langle \phi_{n+1} | \phi_{n+1}\rangle \\ &\quad + \sum_{k=1}^{n} \rho_k \langle \psi_k | \phi_{n+1}\rangle + \sum_{k=1}^{n} \rho_k^* \langle \phi_{n+1} | \psi_k\rangle\Big\} \end{aligned}$$

fixes the constant C. This completes the proof of the Gramm-Schmidt process.

In particular, for any subspace S of dimension M in a larger dimensional space we can find an orthonormal set in which the first

M vectors are in S.

Examples of Discrete Bases:

1) R^3 has basis vectors $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$
$\{\hat{i}, \hat{j}, \hat{k}\}$

so that $\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$. In Dirac notation we write $\hat{e}_1 = |e_1\rangle$, $\hat{e}_2 = |e_2\rangle$, $\hat{e}_3 = |e_3\rangle$ and their orthonormality as

$$\langle e_i | e_j \rangle = \delta_{ij} \; (= \hat{e}_i \cdot \hat{e}_j).$$

Any vector $|v\rangle$ in R^3 has the unique expansion in terms of $\{|e_i\rangle\}$

$$(\vec{v} =)\; |v\rangle = \sum_{i=1}^{3} v_i |e_i\rangle \quad \text{where}$$

$v_i = \langle e_i | v \rangle$. Hence the dot product of $\vec{v}$ and $\vec{u} (= |u\rangle)$ is

$$(\vec{v} \cdot \vec{u} =)\; \langle v | u \rangle = \sum_{i=1}^{3} v_i u_i .$$

---

2) In wavefunction space $L^2(\mathbb{R}^3)$ we have come across several basis. In particular we had the energy eigenfunction basis (ex. Hermite-polynomials)

$$H\psi_n(\vec{r}) = E_n \psi_n(\vec{r}) \quad n = 0,1,2,\ldots$$

Then $\psi(\vec{r}) = \sum_n' c_n \psi_n(\vec{r})$ for any wavefunction. The inner product was given by

$$\langle \psi | \psi_n \rangle \equiv \int d^3r\, \psi^*(\vec{r}) \psi_n(\vec{r})$$

and for orthonormal $|\psi_n\rangle$ we have

$$\langle \psi_n | \psi_m \rangle = \int d^3r\, \psi_n^*(\vec{r}) \psi_m(\vec{r}) = \delta_{mn}$$

and

$$c_n = \langle \psi_n | \psi \rangle = \int d^3r\, \psi_n^*(\vec{r}) \psi(\vec{r}).$$

Further for another wavefunction $\phi(\vec{r})$

$$\phi(\vec{r}) = \sum_n' d_n \psi_n(\vec{r}) \quad \text{we have}$$

$$\langle \phi | \psi \rangle = \sum_n' d_n^* c_n .$$

Continuous Orthonormal Basis in $\hat{\mathcal{H}}$:

When we include vectors labelled by a continuous index in our space, we have bases sets of such vectors for $\mathcal{H}$. Their properties are analogous to the discrete index bases of $\mathcal{H}$.

If $\{|\phi_\alpha\rangle\}$ is a complete orthonormal basis depending on a continuous parameter α, then any arbitrary ket vectors $|\psi\rangle, |\phi\rangle$ can be written as

$$|\psi\rangle = \int d\alpha\, \psi(\alpha)\, |\phi_\alpha\rangle$$

$$|\phi\rangle = \int d\alpha\, \phi(\alpha)\, |\phi_\alpha\rangle .$$

Since

$$\langle \phi_\alpha | \phi_\beta \rangle = \delta(\alpha - \beta),$$ due to

the orthonormal continuum normalization, we have

$$\psi(\alpha) = \langle \phi_\alpha | \psi \rangle = \int d\beta\, \psi(\beta) \overbrace{\langle \phi_\alpha | \phi_\beta \rangle}^{=\delta(\alpha-\beta)} .$$

Likewise the inner product between

$|\psi\rangle$ and $|\phi\rangle$ becomes

$$\langle\psi|\phi\rangle = \int d\alpha\, d\beta\, \psi^*(\alpha)\, \phi(\beta) \langle\phi_\alpha|\phi_\beta\rangle$$
$$= \int d\alpha\, d\beta\, \psi^*(\alpha)\, \phi(\beta)\, \delta(\alpha-\beta)$$
$$= \int d\alpha\, \psi^*(\alpha)\, \phi(\alpha) .$$

and the norm of a element of $\underline{\underline{\mathcal{H}}}$ becomes

$$\langle\psi|\psi\rangle = \int d\alpha\, \psi^*(\alpha) \psi(\alpha) .$$

<u>examples:</u> i) Clearly our plane-wave states have been such a set of basis vectors. Any wavefunction $\psi(\vec{r})$ can be expanded in terms of them

$$\psi(\vec{r}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, \tilde{\psi}(\vec{k})$$

and defining $u_{\vec{k}}(\vec{r}) \equiv e^{i\vec{k}\cdot\vec{r}}$ as the continuum indexed basis vectors we have

$$\langle u_{\vec{k}} | u_{\vec{\ell}} \rangle = \delta^3(\vec{k}-\vec{\ell})\,(2\pi)^3$$
$$= \int d^3r\, u^*_{\vec{k}}(\vec{r})\, u_{\vec{\ell}}(\vec{r}) .$$

2) Another example of continuum labelled basis vectors are given by the position eigenfunctions $\{\varphi_{\vec{r}_0}\}$

$$\varphi_{\vec{r}_0}(\vec{r}) = \delta^3(\vec{r}-\vec{r}_0) .$$

They are complete, recall, since

$$\int d^3r_0 \, \varphi^*_{\vec{r}_0}(\vec{r})\varphi_{\vec{r}_0}(\vec{r}\,') = \delta^3(\vec{r}-\vec{r}\,'),$$

and continuum orthonormal

$$\int d^3r \, \varphi^*_{\vec{r}_0}(\vec{r})\varphi_{\vec{r}_0'}(\vec{r}) = \delta^3(\vec{r}_0-\vec{r}_0\,').$$

Any wavefunction $\psi(\vec{r})$ can be expanded in terms of them

$$\psi(\vec{r}) = \int d^3r_0 \, f(\vec{r}_0)\varphi_{\vec{r}_0}(\vec{r}) .$$

Here we have

$$\langle\varphi_{\vec{r}_0}|\psi\rangle = \int d^3r \, \varphi^*_{\vec{r}_0}(\vec{r})\psi(\vec{r}) = \psi(\vec{r}_0)$$

but also

$$= \int d^3r \int d^3r_0' \, f(\vec{r}_0\,')\,\varphi^*_{\vec{r}_0}(\vec{r})\varphi_{\vec{r}_0'}(\vec{r})$$

$$= \int d^3r_0' \, f(\vec{r}_0\,')\,\delta^3(\vec{r}_0-\vec{r}_0\,')$$

$$= f(\vec{r}_0) .$$