IV.) The Abstract Formulation of Quantum Mechanics

4.1) Hilbert Space and Dirac bra-ket notation

Wavemechanics: $\rho = |\psi|^2$ is the position probability density, hence ψ must be square integrable. By the principle of superposition if ψ_1 and ψ_2 are wavefunctions then $\psi_1 + \psi_2$ is a wavefunction! Hence $\psi_1+\psi_2$ must be square-integrable.

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

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

So $|\psi_1+\psi_2|^2 \le |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2|$

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

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

$$\le 2|\psi_1|^2 + 2|\psi_2|^2 .$$

4.1) So, If ψ_1, ψ_2 are square-integrable

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

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

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

Hence $\psi_1 + \psi_2$ is also square-integrable.

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

A <u>complex vector space</u> $\underline{\mathcal{V}}$ 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 $\lambda \in \mathbb{C}$. Also, the vector addition and multiplication of a vector by a complex number obey

4.1)

$$\psi+\phi=\phi+\psi$$ vector addition is commutative

$$\psi+(\phi+\chi)=(\psi+\phi)+\chi$$ associative wrt vector addition

$$\lambda(\phi+\psi)=\lambda\phi+\lambda\psi$$ distributive wrt vector addition

$$(\lambda+\omega)\phi=\lambda\phi+\omega\phi$$ distributive wrt scalar addition

$$\lambda(\omega\phi)=(\lambda\omega)\phi$$ associative wrt scalar multiplication

where ψ, ϕ, χ are vectors and the scalars $\lambda, \omega \in \mathbb{C}$.

Also, there exists a unique vector $\underline{0}$ for which

Vector zero $\longrightarrow$ $$\underline{0}+\psi=\psi$$

$$0\psi=\underline{0}$$ $\longleftarrow$ Vector zero

number zero

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

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

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

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

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

In addition to the above properties which define a complex vector space, such a space may also allow a scalar product or inner product, denoted (ϕ, ψ), to be defined on it with the

4.1) 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 linear in the second entry

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

but anti-linear 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

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

4.1) <u>Proof</u>: Consider the vector $\psi = \psi_1 + \lambda \psi_2$ with $\lambda \in \mathbb{C}$ an arbitrary complex number. Then by the definition of the inner product

$$(\psi,\psi) \geq 0 \quad \Rightarrow$$

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

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

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

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

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

4.1) 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 this above

$$F(\lambda_{min},\lambda_{min}^*) \geq 0$$ yields the Schwarz inequality

$$F(\lambda_{min},\lambda_{min}^*) = (\psi_1,\psi_1) - \frac{(\psi_2,\psi_1)}{(\psi_2,\psi_2)}(\psi_1,\psi_2)$$

$$- \frac{(\psi_1,\psi_2)}{(\psi_2,\psi_2)}(\psi_2,\psi_1) + \frac{(\psi_1,\psi_2)(\psi_2,\psi_1)^*}{(\psi_2,\psi_2)^2}(\psi_2,\psi_2)$$

$$= (\psi_1,\psi_1) - \frac{|(\psi_1,\psi_2)|^2}{(\psi_2,\psi_2)} - \frac{|(\psi_1,\psi_2)|^2}{(\psi_2,\psi_2)} + \frac{|(\psi_1,\psi_2)|^2}{(\psi_2,\psi_2)} \geq 0$$

$$\Rightarrow \boxed{|(\psi_1,\psi_2)|^2 \leq (\psi_1,\psi_1)(\psi_2,\psi_2)}$$

The equality sign holds iff $(\psi,\psi) = 0$, that is $\psi_1 = -\lambda\psi_2$, that's ψ_1 and ψ_2 are multiples of each other ("parallel").

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

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

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

<u>Examples</u>: 1) 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

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

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

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

This set of n-tuples forms a vector space follows from the fact that the sum of 2 n-tuples that obey the finite norm sum is also a finite norm sum n-tuple.

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

then

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

$$\left(\text{Since } \mathrm{Re}\, z \le |z|\right) \quad \le \sum_{i=1}^{n} \left(|z_i|^2 + |w_i|^2 + 2|z_i||w_i| \right)$$

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

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

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

4.1.) 2.) The inner product is given by

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

where $z = (z_1, z_2, \ldots, z_n)$; $w = (w_1, w_2, \ldots, w_n)$.

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 vector is given by

4.1) 2.)

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

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

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

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

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

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

But the Schwarz inequality yields

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

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

4.1) 2) So

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

Hence $\boxed{\|w+z\| \le \|w\| + \|z\|}$

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.

the equality holds only if $w=0$ or $w=\lambda z$ with $\lambda \ge 0$.

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

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

4.1)

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

By the Schwarz inequality: $|(\psi,\phi)| \le \|\psi\|\,\|\phi\|$

So $\|\psi+\phi\|^2 \le \|\psi\|^2 + \|\phi\|^2 + 2\|\psi\|\,\|\phi\|$

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

Hence the $\boxed{\text{triangle inequality} \quad \|\psi+\phi\| \le \|\psi\| + \|\phi\|}$

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, thus

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

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

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 $\lambda \ge 0$.

4.1) 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

$$d(\psi,\phi) \equiv \|\psi-\phi\|,$$

the distance, $d(\psi,\phi)$, 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.

4.1.) 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

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

Using the triangle inequality

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

where m & n independently go to ∞.

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

is called a <u>Cauchy Sequence</u>.

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

A metric space is called <u>complete</u> 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 <u>Hilbert space</u>, 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 $\psi \in \mathcal{H}$,

$$\lim_{n\to\infty} \psi_n = \psi , \quad \text{that is}$$

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

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

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

(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 as an exercise to show that $L^2(\mathbb{R}^3)$ is complete and hence a Hilbert space. That is 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 $\int d^3r\, |\psi(\vec{r})|^2 < \infty$.

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

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

Hilbert space.

First, 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 $(z^{(1)},z^{(2)},\dots)$,

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

converges to 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

4.1) 2.) of the complex (real) numbers.

So the space of finite norm n-tuples of complex numbers is a Hilbert space for n-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 using the position probability amplitude $\psi(\vec{r})$ to describe the system, we could determine all physical quantities from the momentum probability amplitude

$$\varphi(\vec{k}) = \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} \psi(\vec{r})$$

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