

Wave function:  $\psi(t, \vec{x})$ .  $\psi(0, \vec{x}) = f(\vec{x})$  is the w.f. at the time  $t=0$ .

$$\int_{-\infty}^{\infty} |\psi(t, \vec{x})|^2 d^3x = 1 \quad \forall t$$

Mathematically, we are interested in functions which have a finite integral-squared:

$$f(\vec{x}) / \int |f(\vec{x})|^2 d^3x < \infty$$

This function belongs to  $L^2 \equiv L^2(\mathbb{R}^3)$ .

$$f_1(\vec{x}), f_2(\vec{x}) \in L^2 \rightarrow (f_1, f_2) = \int d^3x f_1^*(\vec{x}) f_2(\vec{x})$$

This is a scalar product.

$\left\{ \psi_m \right\}$  ON basis (for instance, eigenstates of  $\hat{A}$  /  $\hat{A}\psi_m = \lambda_m \psi_m$ )

$$f(\vec{x}) = \sum_{m=1}^{\infty} c_m \psi_m \quad (|c_m|^2 \text{ prob. to find } \lambda_m \text{ by measuring } \hat{A})$$

$$(\psi_m, \psi_n) = \int d^3x \psi_m^* \psi_n = \delta_{mn}$$

We have now a "slight" change of notation.

$f_1(\vec{x}) \leftrightarrow |f_1\rangle$  This is called "ket".

There is a univocal correspondence between  $f_1(\vec{x})$  and  $|f_1\rangle$

$|f_1\rangle$  is an element of an Hilbert-space. An Hilbert space is a vectorial space with an infinity of dimension. It is nothing else than the  $L^2$  space.

Heisenberg: 1925. Matrix-formalism of QM. Much more "concrete".

Schrödinger-eq deals with "function" and "diff. eq."

but Heisenberg approach with rather difficult mathematical concepts (in particular at that time).

Hilbert  $\rightarrow$  mathematician, who played an important role in both math and physics.

Physical content of Schrödinger and Heisenberg approaches is exactly the same.

Need of time to understand it and fully digest.

Why? Much more practical in the treatment of QM!! It is in many cases a technical, and also conceptual, help.

$$f_1(\vec{x}) \leftrightarrow |f_1\rangle$$

$$f_2(\vec{x}) \leftrightarrow |f_2\rangle$$

...

$$L^2 \leftrightarrow \mathcal{H}$$

$$\{f_1(\vec{x}), f_2(\vec{x}), \dots\} \quad \{|f_1\rangle, |f_2\rangle, \dots\}$$

$$\int |f_i(\vec{x})|^2 dx < \infty \quad \langle f_i | f_i \rangle \text{ is finite.}$$

$$\langle f_1 | f_2 \rangle = (f_1(\vec{x}), f_2(\vec{x})) = \int f_1^*(\vec{x}) f_2(\vec{x}) d^3x$$

Just a different notation for the scalar product!

Note,  $|f_1\rangle$  is a state!!! It is called ket.

Indeed,  $\langle f_1 |$  is a "bra". strictly speaking, it is an operator:

$$\langle f_1 | : \mathcal{H} \mapsto \mathbb{C}$$

(Note: it is possible to introduce it in the  $(\cdot, \cdot)$  formalism of  $L^2$ , but it would have been more complicated)

Namely:

$$\langle f_1 | : f_2(\vec{x}) \rightarrow \langle f_1 | f_2 \rangle = (f_1, f_2) \in \mathbb{C}$$

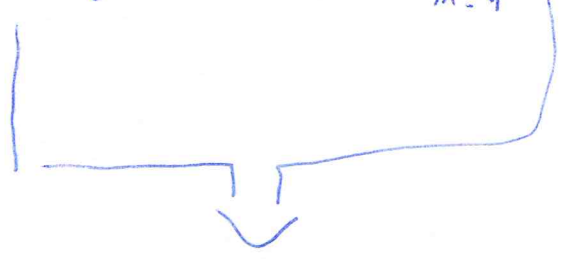
Note:

$$\langle f_1 | f_1 \rangle = (f_1(\vec{x}), f_1(\vec{x})) = \int |f_1(\vec{x})|^2 d^3x \quad (< \infty)$$

Basis  $\{\psi_m(\vec{x})\}$  of  $L^2 \leftrightarrow$  basis  $\{|\psi_m\rangle\}$  of  $\mathcal{H}$

$$(\psi_m(\vec{x}), \psi_n(\vec{x})) = \delta_{nm} = \langle \psi_m | \psi_n \rangle$$

$$\text{Each } f(\vec{x}) / |f\rangle = \sum_{m=1}^{\infty} c_m \psi_m \Leftrightarrow |f\rangle = \sum_{m=1}^{\infty} c_m |\psi_m\rangle$$



These are the very same constants!

$$c_m = (\psi_m(\vec{x}), f(\vec{x})) = \langle \psi_m | f \rangle$$

Important property of a complete basis of  $\mathcal{H}$ :

$$(x) \sum_{m=1}^{\infty} |\psi_m\rangle \langle \psi_m| = 1 \text{ (identity operator)!}$$

Namely:

$$\underbrace{\left[ \sum_{m=1}^{\infty} |\psi_m\rangle \langle \psi_m| \right]}_{\text{operator} = 1} (|f\rangle) = \sum_{m=1}^{\infty} |\psi_m\rangle \overbrace{\langle \psi_m | f \rangle}^{c_m} = \sum_{m=1}^{\infty} c_m |\psi_m\rangle = |f\rangle !!!$$

qed.

$$1|f\rangle = |f\rangle!$$

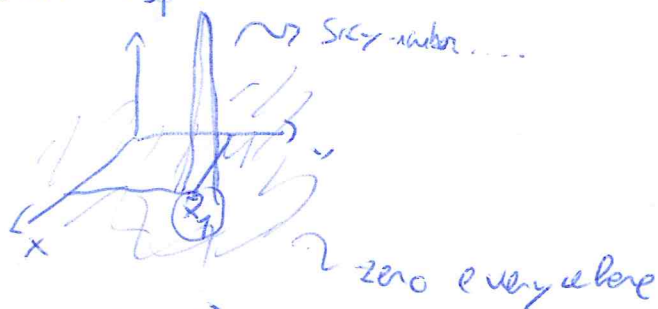
(x) Completeness relation: it holds only if all elements of the basis are included... otherwise I could not reconstruct  $|f\rangle$  (No identity). Also this would be possible within  $L^2$  but it would be more complicated.



What about the position " $\vec{x}_1$ "?

Ante with a definite position  $\vec{x}_1$  has a wave function

$$\psi_{\vec{x}_1}(\vec{x}) = N \delta(\vec{x} - \vec{x}_1)$$



$|\vec{x}_1\rangle \rightarrow$  particle with definite position  $\vec{x}_1$ .

$$\left\{ \begin{array}{l} \{ |\vec{x}\rangle \} / \langle \vec{x}_1 | \vec{x}_2 \rangle = \delta(\vec{x}_1 - \vec{x}_2) \quad \text{ON condition} \\ \left( \sum_{\vec{x}} |\vec{x}\rangle \langle \vec{x}| \right) = \int d^3x |\vec{x}\rangle \langle \vec{x}| = 1 \quad \text{completeness} \end{array} \right.$$

completeness of states

$$\begin{aligned} f(\vec{x}) \mapsto |f\rangle &= 1 \cdot |f\rangle = \int d^3x |\vec{x}\rangle \langle \vec{x}| f\rangle = \\ &= \int d^3x f(\vec{x}) \cdot |\vec{x}\rangle \end{aligned}$$

Indeed, this expression is intuitive: the state  $|f\rangle$  is the superposition of many states  $|\vec{x}\rangle$  with definite positions.

$$\langle f | f \rangle = \int d^3x |f(\vec{x})|^2 = (f(\vec{x}), f(\vec{x}))$$

$$\langle f_1 | f_2 \rangle = \int d^3x f_1^*(\vec{x}) f_2(\vec{x}) = (f_1(\vec{x}), f_2(\vec{x}))$$

States with definite momentum:

$|\vec{k}_1\rangle$  describes a particle with momentum  $\vec{k}_1$ .

$$\text{The w.f. is: } \phi_{\vec{k}_1}(\vec{x}) = N e^{i\vec{k}_1 \cdot \vec{x}} \quad N = \frac{1}{(2\pi)^{3/2}}$$

Ergo:

$$\langle \vec{x} | \vec{k}_1 \rangle = \phi_{\vec{k}_1}(\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}_1 \cdot \vec{x}}$$

$$\left\{ \begin{aligned} \langle \vec{k}_1 | \vec{k}_2 \rangle &= \int d^3x \phi_{\vec{k}_1}^*(\vec{x}) \phi_{\vec{k}_2}(\vec{x}) = \int \frac{d^3x}{(2\pi)^3} e^{i(\vec{k}_2 - \vec{k}_1) \cdot \vec{x}} = \delta^{(3)}(\vec{k}_1 - \vec{k}_2) \\ \langle \vec{k}_1 | \vec{k}_2 \rangle &= \delta^{(3)}(\vec{k}_1 - \vec{k}_2) \end{aligned} \right.$$

$$\begin{aligned} \int d^3k |\vec{k}\rangle \langle \vec{k}| &= \int d^3k |1\rangle \langle 1| = 1 \\ &= \int d^3k \left( \int d^3x_1 |\vec{x}_1\rangle \langle \vec{x}_1 | \vec{k}\rangle \right) \left( \int d^3x_2 \langle \vec{k} | \vec{x}_2\rangle \langle \vec{x}_2 | \right) \\ &= \int d^3x_1 \int d^3x_2 |\vec{x}_1\rangle \langle \vec{x}_2 | \underbrace{\left( \int d^3k \langle \vec{x}_1 | \vec{k}\rangle \langle \vec{k} | \vec{x}_2\rangle \right)}_{\delta^3(\vec{x}_1 - \vec{x}_2)} \\ &= \int d^3x_1 |\vec{x}_1\rangle \langle \vec{x}_1 | = 1 \end{aligned}$$

As a consequence, it follows that each state  $|f\rangle$  can (7) be expressed in the basis  $\{|\vec{k}\rangle\}$ :

$$|f\rangle = \int d^3\vec{k} \underbrace{\langle \vec{k} | f \rangle}_{A(\vec{k})} |\vec{k}\rangle = \int d^3\vec{k} A(\vec{k}) |\vec{k}\rangle.$$

Note, being:

$$|\vec{k}\rangle = \int d^3\vec{x} \langle \vec{x} | \vec{k} \rangle |\vec{x}\rangle = \int d^3\vec{x} \frac{1}{(2\pi)^3} e^{-i\vec{k}\vec{x}} |\vec{x}\rangle$$

$$|f\rangle = \int d^3\vec{k} \int d^3\vec{x} \frac{1}{(2\pi)^{3/2}} e^{-i\vec{k}\vec{x}} |\vec{x}\rangle =$$

$$= \int d^3\vec{x} \left[ \int \frac{d^3\vec{k}}{(2\pi)^{3/2}} A(\vec{k}) e^{-i\vec{k}\vec{x}} \right] |\vec{x}\rangle$$

$$f(\vec{x}) = \int \frac{d^3\vec{k}}{(2\pi)^{3/2}} A(\vec{k}) e^{-i\vec{k}\vec{x}}$$

fourier-transform of  $A(\vec{k})$ .

$|f\rangle$  expressed in the basis of  $|\vec{x}\rangle \mapsto f(\vec{x})$  (d.f. in position space)

$|f\rangle$  " " " " "  $|\vec{k}\rangle \mapsto A(\vec{k})$  (d.f. in momentum space)

DEFINITIONS

Operator:  $\hat{A}_{\vec{x}} : L^2 \mapsto L^2$

↳ it is now important to specify it. (Before it was always like  $\hat{p}$ )

$\Rightarrow \hat{A}_{\vec{x}} = i\vec{x} \cdot \frac{\partial}{\partial \vec{y}}$  is an example of a Hermitian operator  
( $-i\vec{x} \cdot \vec{p}$ ).

$f(\vec{x}) \in L^2$

$\hat{A}_{\vec{x}} f(\vec{x}) = g(\vec{x}) \in L^2$

How does it translate it in the Hilbert space  $\mathcal{F}$ ?

$f(\vec{x}) \mapsto |f\rangle$

$g(\vec{x}) \mapsto |g\rangle$

$\hat{A}_{\vec{x}} \mapsto A \cdot \mathcal{F} \mapsto \mathcal{F}$  such that

$A|f\rangle = |g\rangle$   
 $A|f\rangle = |\hat{A}_{\vec{x}} f\rangle = |g\rangle$

$A|f\rangle = A\left(\int d^3x \langle \vec{x}|f\rangle |\vec{x}\rangle\right) = \int d^3x f(\vec{x}) \cdot A|\vec{x}\rangle$

But  $A|f\rangle = |g\rangle$

Then:

$\langle \vec{x}'|A|f\rangle = g(\vec{x}') = \int d^3x f(\vec{x}) \langle \vec{x}'|A|\vec{x}\rangle$

Ergo:

$\langle \vec{x}'|A|\vec{x}\rangle = \delta(\vec{x}-\vec{x}') A_{\vec{x}'}$



Wave function  $\Psi(t, \vec{x})$

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}_{\vec{x}} \Psi = \left( -\frac{\hbar^2}{2m} \Delta + V(\vec{x}) \right) \Psi$$

$$\Psi(t, \vec{x}) \in L^2 \quad \forall t.$$

Then  $\Psi(t, \vec{x}) \mapsto |\Psi(t)\rangle$ .

The Schrödinger eq.

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle$$

$$\Psi(0, \vec{x}) = \Psi_0(\vec{x})$$

$$|\Psi(t)\rangle = e^{-iHt/\hbar} |\Psi_0\rangle$$

formal sol. of the eq. of Schrödinger.

Proof:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = i\hbar \left( -\frac{iH}{\hbar} \right) e^{-iHt/\hbar} |\Psi_0\rangle = H |\Psi(t)\rangle.$$

Note:

$H$  is Hermitian,  $H^\dagger = H$ .

$U_T = e^{-iHT/\hbar}$  is the Time-evolution operator.

This is a unitary operator:

$$U_T^\dagger = e^{iHT/\hbar} = U_T^{-1}$$

$$U_T^\dagger U_T = U_T U_T^\dagger = 1.$$

Example

$$\{ |1\rangle, |2\rangle, |3\rangle \} \quad H|m\rangle = E_m |m\rangle$$

$$\langle m|m\rangle = \delta_{mm}$$

is the state  $|5\rangle = |1\rangle + |2\rangle + |3\rangle$  physical?

Answer: NO!

$$\begin{aligned} \langle 5|5\rangle &= (\langle 1| + \langle 2| + \langle 3|)(|1\rangle + |2\rangle + |3\rangle) = \\ &= \langle 1|1\rangle + \langle 2|2\rangle + \langle 3|3\rangle = 1 + 1 + 1 = 3. \\ &\neq 1. \end{aligned}$$

A physical state is an element of  $\mathcal{F}$  such that  $\langle 5|5\rangle = 1$ .

Note: strictly speaking  $|5\rangle$  is not uniquely defined. Namely:  $|5\rangle$  and  $e^{i\phi}|5\rangle$  describe the same state

(just as  $\psi(t, \vec{x})$  and  $e^{i\phi}\psi(t, \vec{x})$  are the very same description of a physical particle).

$$\bullet |5\rangle = |1\rangle$$

↳ physical? Yes.  $\langle 5|5\rangle = 1$ .

$$\bullet |5\rangle = e^{i\phi_1} |1\rangle$$

$$\langle 5|5\rangle = \langle 1| e^{-i\phi_1} \cdot e^{i\phi_1} |1\rangle = 1 \text{ also.}$$

Adding:

$$\langle 5| = \langle 1| e^{-i\phi_1}$$

$$\bullet \text{ In general: } |5\rangle = a |1\rangle$$

$$\langle 5| = \langle 1| a^*$$

$$\bullet |5\rangle = \frac{e^{i\phi_1}}{\sqrt{3}} |1\rangle + \frac{e^{i\phi_2}}{\sqrt{3}} |2\rangle + \frac{e^{i\phi_3}}{\sqrt{3}} |3\rangle$$

$$\langle 5|5\rangle = \left( \frac{e^{-i\phi_1}}{\sqrt{3}} \langle 1| + \frac{e^{-i\phi_2}}{\sqrt{3}} \langle 2| + \frac{e^{-i\phi_3}}{\sqrt{3}} \langle 3| \right) \left( \frac{e^{i\phi_1}}{\sqrt{3}} |1\rangle + \frac{e^{i\phi_2}}{\sqrt{3}} |2\rangle + \frac{e^{i\phi_3}}{\sqrt{3}} |3\rangle \right) = 1$$

Prob. of energy:

$\frac{1}{3}$  to find  $E_1$ ,  $\frac{1}{3}$  to find  $E_2$ ,  $\frac{1}{3}$  to find  $E_3$ .

## Average of an operator

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$$t=0$$

$|\psi\rangle$ , operator  $A$

$\langle \psi | \hat{A} | \psi \rangle$  is the average!

=

in our case:

$$|\psi\rangle = \frac{e^{i\phi_1}}{\sqrt{3}} |1\rangle + \frac{e^{i\phi_2}}{\sqrt{3}} |2\rangle + \frac{e^{i\phi_3}}{\sqrt{3}}$$

$$\langle \psi | \hat{H} | \psi \rangle = \frac{E_1}{3} + \frac{E_2}{3} + \frac{E_3}{3}$$



Which is the probability to find the state  $|s\rangle$  as described as  $\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$  by a measurement of the state?

This is equivalent to a measurement of the operator

$$\hat{A} = |a\rangle\langle a|$$

$$\text{with } |a\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle).$$

$$\langle s|A|s\rangle = \left( \frac{e^{-i\phi_1}}{\sqrt{3}} \langle 1| + \frac{e^{-i\phi_2}}{\sqrt{3}} \langle 2| + \frac{e^{-i\phi_3}}{\sqrt{3}} \langle 3| \right)$$

$$|a\rangle\langle a|s\rangle = |\langle a|s\rangle|^2$$

$$\langle a|s\rangle = \frac{1}{\sqrt{2}} \left( \langle 1| + \langle 2| \right) \left( \frac{e^{-i\phi_1}}{\sqrt{3}} |1\rangle + \frac{e^{-i\phi_2}}{\sqrt{3}} |2\rangle + \frac{e^{-i\phi_3}}{\sqrt{3}} |3\rangle \right)$$

$$= \frac{1}{\sqrt{6}} e^{-i\phi_1} + \frac{1}{\sqrt{6}} e^{-i\phi_2}$$

$$\text{Prob: } |\langle a|s\rangle|^2 = \frac{1}{6} \left| e^{-i\phi_1} + e^{-i\phi_2} \right|^2 = \frac{1}{6} (2 + 2\cos(\Delta\phi))$$

$\{|1\rangle, |2\rangle\}$  basis.

$$\begin{aligned} \langle 1|1\rangle &= 1 \\ \langle 1|2\rangle &= \langle 2|1\rangle \\ \langle 2|2\rangle &= 0 \end{aligned}$$

$$H|1\rangle = E_1|1\rangle$$

$$H|2\rangle = E_2|2\rangle$$

$H = ?$

$$H = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$$

In fact:

$$H|1\rangle = (E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|)|1\rangle = E_1|1\rangle \quad \text{q.e.d.}$$

$$|\psi(t)\rangle \text{ with } |\psi(0)\rangle = a|1\rangle + b|2\rangle \quad |a|^2 + |b|^2 = 1$$

The Schrödinger eq is:

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H |\psi(t)\rangle$$

$$\begin{aligned} |\psi(t)\rangle &= e^{-iHt/\hbar} |\psi(0)\rangle = e^{-iHt/\hbar} (a|1\rangle + b|2\rangle) = \\ &= a e^{-iE_1 t/\hbar} |1\rangle + b e^{-iE_2 t/\hbar} |2\rangle = \\ &= |\psi(t)\rangle \end{aligned}$$

In general:

$$H|1\rangle = E_1|1\rangle$$

$$\left[ f(H)|1\rangle = f(E_1)|1\rangle \right]$$

In fact:

$$e^{-iHt/\hbar} |1\rangle = e^{-iE_1 t/\hbar} |1\rangle$$