* lecture 7 *

- discrete spectrum -	- continuous spectrum -
$\hat{f}\,\psi_n(q) = f_n\,\psi_n(q)$	$\longrightarrow$ $\hat{f}\,\psi_f(q) = f\,\psi_f(q)$
$(n=1,2,\ldots)$ discrete label	$f \in \mathbb{R}$ continuous label
$\psi(q) = \sum_n a_n\,\psi_n(q)$	$\longrightarrow$ $\psi(q) = \int a_f\,\psi_f(q)\,df$ (0)

As f denotes a continuous label is more convenient to write it in the argument of the function, as a real-valued parameter, namely:

$$\psi_f(q) \to \phi(q,f) \quad \text{and} \quad a_f \to a(f)$$

In the discrete case, from the normalization condition

$$\int \psi^*\psi\, dq = 1 \qquad (1)$$

we deduced that

$$\sum_n |a_n|^2 = 1 \qquad (2)$$

In the continuous case, (1) is not altered, by (2) must be replaced by:

$$\sum_n |a_n|^2 = 1 \longrightarrow \int \underbrace{|a(f)|^2 df}_{} = 1$$

= Probability that a measure of f upon the system prepared in the state ψ, gives a value between f and $f+df$.

We use the equality

$$\int \psi^* \psi \, dq = 1 = \int |a(f)|^2 df \quad (3)$$

to find the expression for $a(f)$.

$$\int \psi^* \psi \, dq = \int \left(\int a(f) \phi(q,f) \, df \right)^* \psi(q) \, dq$$

$$= \iint a^*(f) \phi^*(q,f) \psi(q) \, df \, dq$$

$$= \int a^*(f) \left[\int \phi^*(q,f) \psi(q) \, dq \right] df$$

(from (3)) $$= \int a^*(f) a(f) \, df \Rightarrow$$

$$\Rightarrow \boxed{a(f) = \int \phi^*(q,f) \psi(q) \, dq} \quad (4)$$

Also the orthogonality condition $\int \psi_n^* \psi_m \, dq = \delta_{nm}$ changes in the transition from the discrete to the continuous case. To see this, substitute in (4) ψ with its expression (0):

$$\boxed{\psi(q) = \int a(f) \phi(q,f) \, df} \quad (4b)$$

to obtain:

$$a(f) = \int \phi^*(q,f) \left[\int a(g) \phi(q,g) \, dg \right] dq$$

$$Q(f) = \int a(g) \left[\int \phi^*(q,f)\, \phi(q,g)\, dq \right] dg \Rightarrow$$

$$\Rightarrow \boxed{\int \phi^*(q,f)\, \phi(q,g)\, dq = \delta(g-f)}$$

ORTHOGONALITY RELATION (5)

Finally, the completeness relation becomes:

$$\Psi(q) = \int \underbrace{a(f)}_{\text{replace with (4)}} \phi(q,f)\, df$$

$$= \int \left[\int \phi^*(q',f)\, \Psi(q')\, dq' \right] \phi(q,f)\, df$$

change the order of integration

$$= \int \Psi(q') \left[\int \phi(q,f)\, \phi^*(q',f)\, df \right] dq' \Rightarrow$$

$$\Rightarrow \boxed{\int \phi(q,f)\, \phi^*(q',f)\, df = \delta(q'-q)} \quad (6)$$

COMPLETENESS (OR, CLOSURE) RELATION

— Example — Eigenfunction of the position operator.

From postulate III, there must exist an operator $\hat{X}$ such that for a system prepared in the state $\psi(x)$ we have:

"mean position of the particle in the state $\psi(x)$" $= \langle x \rangle_\psi$

and

$$\langle x \rangle_\psi = \int \psi^*(x)\,(\hat{X}\psi)(x)\,dx \qquad (7)$$

On the other hand, we already know that:

"Probability to find the particle between x and $x+dx$" $= P(x)dx$

where

$$P(x) = |\psi(x)|^2$$

Therefore, the expectation value of the random variable x is

$$E[x] = \int_{-\infty}^{\infty} x\,P(x)\,dx$$

$$= \int_{-\infty}^{\infty} x\,|\psi(x)|^2\,dx = \int_{-\infty}^{\infty} \psi^*(x)\,x\,\psi(x)\,dx \qquad (8)$$

Imposing $\langle x \rangle_\psi = E[x]$ we obtain

$$\boxed{\int \psi^*(x)\,(\hat{X}\psi)(x)\,dx = \int \psi^*(x)\,x\,\psi(x)\,dx} \qquad (9)$$

Now, let

$$\phi(x,x')$$

be the (still unknown) eigenfunction of the operator $\hat{x}$; defined as:

$$\boxed{\hat{X}\,\phi(x,x') = x'\,\phi(x,x')} \qquad (10)$$

If we rewrite (9) with $\phi(x,x')$ instead of $\psi(x)$, we obtain

$$\int \phi^*(x,x')\underbrace{\left(\hat{x}\,\phi(x,x')\right)}_{\text{from (10)}\ = x'\phi(x,x')} dx = \int \phi^*(x,x')\, x\, \phi(x,x')\, dx$$

$$\Leftrightarrow \int \phi^*(x,x')\, x'\, \phi(x,x')\, dx = \int \phi^*(x,x')\, x\, \phi(x,x')\, dx$$

$$\Leftrightarrow \int \phi^*(x,x')\left[(x'-x)\,\phi(x,x')\right] dx = 0 \qquad \forall x' \in \mathbb{R}$$

This equality can be satisfied for any value x'! iff

$$(11) \quad \boxed{(x'-x)\,\phi(x,x') = 0} \Rightarrow$$

$$\Rightarrow \phi(x,x') = \begin{cases} \text{"any value"}, & x'-x=0 \\ 0, & x'-x \neq 0 \end{cases}$$

We know that:

$$(x'-x)\,\delta(x'-x)=0 \qquad \forall x,x'\in\mathbb{R}$$

Therefore we try:

$$\phi(x,x')=\lambda\,\delta(x'-x)$$

where $\lambda\in\mathbb{C}$ is a normalization constant that is fixed by the orthogonality relation (5)

that we rewrite as:

$$\underbrace{\int \phi^*(x,x')\,\phi(x,x'')\,dx}=\delta(x''-x')$$

$$=|\lambda|^2\int \delta(x'-x)\,\delta(x''-x)\,dx \;\leftarrow$$ We can integrate either with respect to the first delta or the second one.

$$=|\lambda|^2\,\delta(x''-x') \qquad \Rightarrow |\lambda|^2=1$$

We disregard the phase factor and we choose $\lambda=1$.

This implies:

$$\boxed{\phi(x,x')=\delta(x'-x)} \qquad (12)$$

Note In the function $\phi(x,x')$, the first argument x is the independent variable, while x' is a parameter that characterizes the eigenfunction. In other words, x' plays the role of a label.

HOMEWORK:

Demonstrate that:

$$\frac{\delta(x''-x')}{x''-x'} = \frac{\partial}{\partial x'}\delta(x''-x') = -\frac{\partial}{\partial x''}\delta(x''-x')$$

for any good function $f(x)$. Remember that given two DISTRIBUTION FUNCTIONS (as, e.g., the Dirac delta functions), say F and G, then

$$F = G \quad \text{means} \quad \int F f(x)\,dx = \int G f(x)\,dx$$

In 3D, we have 3 position operators denoted either as $\hat{x}, \hat{y}, \hat{z}$ or $\hat{x}_1, \hat{x}_2, \hat{x}_3$. The eigenfunctions are denoted with

$$\phi(\underline{x}, \underline{x}') \doteq \delta(x_1 - x_1')\,\delta(x_2 - x_2')\,\delta(x_3 - x_3')$$

and

$$\hat{\underline{X}}\,\phi(\underline{x}, \underline{x}') = \underline{x}'\phi(\underline{x}, \underline{x}') \iff \hat{x}_i\,\phi(\underline{x}, \underline{x}') = x_i'\,\phi(\underline{x}, \underline{x}')$$

- Differen coordinate operators commute: $[\hat{x}_i, \hat{x}_j] = 0$

Proof:

$$\hat{x}_j\hat{x}_i\,\phi(\underline{x}, \underline{x}') = \hat{x}_j\,[x_i'\,\phi(\underline{x}, \underline{x}')] = x_i' x_j'\,\phi(\underline{x}, \underline{x}')$$

$$\hat{x}_i\hat{x}_j\,\phi(\underline{x}, \underline{x}') = x_j' x_i'\,\phi(\underline{x}, \underline{x}')$$

c.v.d.

In the general case of the N coordinates

$$q_1, q_2, \dots, q_N$$

of a quantum system, shortly denoted simply with q, we have:

independent variable

$$\hat{q}\,\phi(q, q') = q'\,\phi(q, q')$$

label

where $\phi(q, q') = \delta(q' - q)$

Note This is a short hand for:

$$\hat{q}_i\,\delta(q'_i - q_i) = q'_i\,\delta(q'_i - q_i)$$

According to ④, if $f = q$:

$$a(q) = \int \phi^*(q', q)\,\psi(q')\,dq'$$

$$= \int \delta(q - q')\,\psi(q')\,dq'$$

$$= \psi(q)$$

The coefficient $a(q)$ of the expansion of the wave function $\psi(q)$ in the eigenfunctions of the operator $\hat{q}$, coincide with the wave function $\psi(q)$ itself. Therefore $\psi(q)$ is often denoted as:

$\psi(q)$ = "Wave function of the system in representation q"

We generalize this concept understanding the coefficient $a(f)$ as:

$a(f) =$ "Wave function in representation f"

This interpretation of $a(f)$ makes sense because:

Observable q	Observable f
$P(q)dq = \lvert\psi(q)\rvert^2 dq$ = Probability that the coordinate of the particle lie between q and $q+dq$	$P(f)\,df = \lvert a(f)\rvert^2 df$ = Probability that the values assumed by the observable f belong to the interval $(f, f+df)$
expectation value of $\hat{q}$ – $\langle q\rangle_\psi = \int q\lvert\psi(q)\rvert^2 dq$	expectation value of $\hat{f}$ – $\langle f\rangle_\psi = \int \psi^*(\hat{f}\psi)\,dq$

use (ab)

$$= \int\left\{\left[\int a(f)\phi(q,f)\,df\right]^* \times \hat{f}\left[\int a(f')\phi(q,f')\,df'\right]dq\right.$$

$$= \iint\left\{a^*(f)\,a(f') \times \underbrace{\left[\int \phi^*(q,f)\underbrace{\hat{f}\,\phi(q,f')}_{=f'\phi(q,f')}dq\right]}_{=f'\delta(f-f')}\right\}df\,df'$$

from (5)

$$= \iint a^*(f)\,a(f')\,f'\delta(f-f')\,df\,df'$$

$$= \int f\lvert a(f)\rvert^2 df$$

$$\psi(q) = \int \underbrace{a(f)}_{f\text{-dependent coefficient}} \underbrace{\phi(q,f)}_{\text{basis function}} \, df \quad (4b)$$

– orthogonality –

$$(5) \quad \int \phi^*(q,f)\,\phi(q,f')\,dq = \delta(f'-f)$$

parameters: f, f'; integration variable: q

$$a(f) = \int \underbrace{\psi(q)}_{q\text{-dependent coefficient}} \underbrace{\phi^*(q,f)}_{\text{basis function}} \, dq \quad (4)$$

– orthogonality – (completeness)

$$\int [\phi^*(q,f)]^* \phi^*(q',f)\,df$$

parameters: q, q'

$$= \int \phi(q,f)\,\phi^*(q',f)\,df$$

integration variable: f

$$= \delta(q'-q)$$

If $\phi(q,f)$ are the eigenfunctions of $\hat{f}$ in representation q:

independent variable: q

$$(\hat{f}\phi)(q) = f\,\phi(q,f),$$

label: f

what are the eigenfunctions of $\hat{q}$ in representation f?

independent variable: f

$$(\hat{q}\varphi)(f) = q\,\varphi(f,q) \quad (12b)$$

label: q

From (4) it follows that $\phi^*(q,f)$ must be interpreted as the eigenfunctions of the coordinate q in representation f $\Rightarrow$ $\boxed{\varphi(f,q) = \phi^*(q,f)}$ (13)

Notice that if we make a "restyling" writing

$$\phi_f(q) \quad \text{instead of} \quad \phi(q,f)$$

Then the eigenfunctions of $\hat{q}$ in representation q and f are:

because $\phi_{q'}(q) = \delta(q'-q)$

$$(\hat{q}\,\phi_{q'})(q) = q'\,\phi_{q'}(q) = q\,\phi_q(q') \quad \text{(from page 8)}$$

and

$$(\hat{q}\,\varphi_{q'})(f) = q'\varphi_{q'}(f) \quad \text{(from page 10)}$$

Then

$$\psi(q) = \int \delta(q'-q)\,\psi(q')\,dq'$$

$$= \int \phi_{q'}(q)\,\psi(q')\,dq'$$

and

$$a(f) \equiv \tilde{\psi}(f) = \int \varphi_{q'}(f)\,\psi(q')\,dq'$$

In summary:

$$\psi(q) = \int \phi_{q'}(q)\,\psi(q')\,dq' \iff \langle q| \int |q'\rangle\langle q'|\psi\rangle\,dq'$$

$$\tilde{\psi}(f) = \int \varphi_{q'}(f)\,\psi(q')\,dq' \iff \langle f| \underbrace{\int |q'\rangle\langle q'|\psi\rangle\,dq'}$$

These expressions will make sense in the future lectures. Do not worry about them now.

— Translation and momentum operators —

let $\hat{T}(\underline{\delta})$ be an operator representing the physical operation of translating our system from $\underline{x}$ to $\underline{x}+\underline{\delta}$, where $\underline{\delta}=(\delta_x,\delta_y,\delta_z)$ is a <u>constant</u> real vector.

$$\left(\hat{T}(\underline{\delta})\psi\right)(\underline{x}) = \psi(\underline{x}-\underline{\delta})$$
$$\equiv \phi(\underline{x})$$

To determine $\hat{T}(\underline{\delta})$, we require:

1) The displaced wave function $\phi(\underline{x})$ has the same norm of $\psi(\underline{x})$; namely

$$\int|\phi|^2 d^3x = \int|\psi|^2 d^3x = 1 \quad \Rightarrow$$

$$\Rightarrow \int|\phi|^2 d^3x = \int\left[\hat{T}(\underline{\delta})\psi\right]^*\left[\hat{T}(\underline{\delta})\psi\right]d^3x$$
$$= \int\left(\hat{T}^*(\underline{\delta})\,\psi^*\right)\left(\hat{T}(\underline{\delta})\psi\right)d^3x$$

Remember that:

$$\int u(\hat{f}v)\,dq = \int(\hat{f}v)\,u\,dq = \int v(\hat{f}^T u)\,dq$$

$$\int |\phi|^2 d^3x = \int \psi^* \underbrace{\left[\hat{T}^*(\underline{\delta})\right]^T}_{\equiv \hat{T}^\dagger(\underline{\delta})} \hat{T}(\underline{\delta}) \psi \, d^3x$$

$$= \int \psi^* \left(\hat{T}^\dagger(\underline{\delta}) \hat{T}(\underline{\delta}) \right) \psi \, d^3x$$

impose $= \int |\psi|^2 d^3x \Rightarrow \boxed{\hat{T}^\dagger(\underline{\delta}) \hat{T}(\underline{\delta}) = \hat{I}}$ UNITARY

2) Displacements are additive.

we require $\hat{T}(\underline{\delta})$ to satisfy:

$$\hat{T}(\underline{\delta}'') \hat{T}(\underline{\delta}') = \hat{T}(\underline{\delta}'' + \underline{\delta}')$$

However, since $\underline{\delta}'' + \underline{\delta}' = \underline{\delta}' + \underline{\delta}'' \Rightarrow$

$$\Rightarrow \hat{T}(\underline{\delta}'') \hat{T}(\underline{\delta}') = \hat{T}(\underline{\delta}') \hat{T}(\underline{\delta}'') \Leftrightarrow [\hat{T}(\underline{\delta}''), \hat{T}(\underline{\delta}')] = 0$$

3) If $\underline{\delta} = \underline{0}$, $\hat{T}(\underline{0}) = \hat{I}$ because:

$$\left(\hat{T}(\underline{\delta} = 0)\psi\right)(\underline{x}) = \psi(\underline{x} + \underline{0}) = \psi(\underline{x})$$

4) A negative displacement is realized by the inverse operator.

$$\underline{\delta} + (-1)\underline{\delta} = \underline{0} \Rightarrow$$

$$\Rightarrow \hat{I} = \hat{T}(\underline{0}) = \hat{T}(\underline{\delta} + (-\underline{\delta})) = \hat{T}(-\underline{\delta}) \hat{T}(\underline{\delta}) = \hat{T}(\underline{\delta}) \hat{T}(-\underline{\delta})$$

Therefore $\boxed{\hat{T}^{-1}(\underline{\delta}) = \hat{T}(-\underline{\delta})}$

If $|\underline{\delta}| \ll 1$, These properties are approximatively realized by an operator of the form:

$$\hat{T}(\underline{\delta}) \simeq \hat{I} - i\,\underline{\hat{K}}\cdot\underline{\delta} + O(\underline{\delta}^2)$$
$$= \hat{I} - i\hat{K}_x\delta_x - i\hat{K}_y\delta_y - i\hat{K}_z\delta_z + \cdots$$

1) $\hat{T}^{+}(\underline{\delta})\,\hat{T}(\underline{\delta}) = \hat{I}$

$$[\hat{I} - i\,\underline{\hat{K}}\cdot\underline{\delta}]^{+}[\hat{I} - i\,\underline{\hat{K}}\cdot\underline{\delta}] = (\hat{I} + i\,\underline{\hat{K}}^{+}\cdot\underline{\delta})(\hat{I} - i\,\underline{\hat{K}}\cdot\underline{\delta})$$
$$\simeq \hat{I} - i\,(\underline{\hat{K}} - \underline{\hat{K}}^{+})\cdot\underline{\delta} + O(\underline{\delta}^2) \Rightarrow \boxed{\underline{\hat{K}} - \underline{\hat{K}}^{+} = 0}$$

$\Leftrightarrow$ $\underline{\hat{K}}$ must be an Hermitian operator

2) $$\hat{T}(\underline{\delta}'')\,\hat{T}(\underline{\delta}') = (\hat{I} - i\,\underline{\hat{K}}\cdot\underline{\delta}'')(\hat{I} - i\,\underline{\hat{K}}\cdot\underline{\delta}')$$
$$\simeq \hat{I} - i\,\underline{\hat{K}}\cdot(\underline{\delta}'' + \underline{\delta}') + \cdots$$
$$\simeq \hat{T}(\underline{\delta}'' + \underline{\delta}')$$

3) $$\hat{T}(\underline{0}) = (\hat{I} - i\,\underline{\hat{K}}\cdot\underline{\delta})\big|_{\underline{\delta}=\underline{0}} = \hat{I}$$

4) $$\hat{T}(-\underline{\delta})\,\hat{T}(\underline{\delta}) \simeq \hat{I} - i\,\underline{\hat{K}}\cdot\underbrace{(\underline{\delta} - \underline{\delta})}_{=0} + \cdots \simeq \hat{I} + \cdots$$

The Translation operator DOES NOT COMMUTE with the position operators $\hat{X}_1, \hat{X}_2, \hat{X}_3$.

To see this, let us calculate:

$$\hat{\underline{X}}\left(\hat{T}(\underline{\delta})\,\phi(\underline{X},\underline{x}')\right) = \hat{\underline{X}}\left(\phi(\underline{x}-\underline{\delta},\underline{x}')\right)$$

but
$$\phi(\underline{x}-\underline{\delta},\underline{x}') = \delta(\underline{x}'-\underline{x}+\underline{\delta})$$
$$= \delta\left[(\underline{x}'+\underline{\delta})-\underline{x}\right]$$
$$= \phi(\underline{x},\underline{x}'+\underline{\delta}) \Rightarrow$$

$$\Rightarrow \hat{\underline{X}}\left(\phi(\underline{x}-\underline{\delta},\underline{x}')\right) = \hat{\underline{X}}\,\phi(\underline{x},\underline{x}'+\underline{\delta})$$
$$= (\underline{x}'+\underline{\delta})\,\phi(\underline{x},\underline{x}'+\underline{\delta})$$

On the other hand:

$$\hat{T}(\underline{\delta})\left(\hat{\underline{X}}\,\phi(\underline{x},\underline{x}')\right) = \underline{x}'\,\hat{T}(\underline{\delta})\,\phi(\underline{x},\underline{x}')$$
$$= \underline{x}'\,\phi(\underline{x}-\underline{\delta},\underline{x}')$$
$$= \underline{x}'\,\phi(\underline{x},\underline{x}'+\underline{\delta})$$

This means that:

$$[\hat{\underline{X}},\hat{T}(\underline{\delta})]\,\phi(\underline{x},\underline{x}') = +\underline{\delta}\,\phi(\underline{x},\underline{x}'+\underline{\delta})$$

Since $\phi(\underline{x},\underline{x}'+\underline{\delta}) \simeq \phi(\underline{x},\underline{x}') + \underline{\delta}\,\phi'(\underline{x},\underline{x}') + O(\underline{\delta}^2) \Rightarrow$

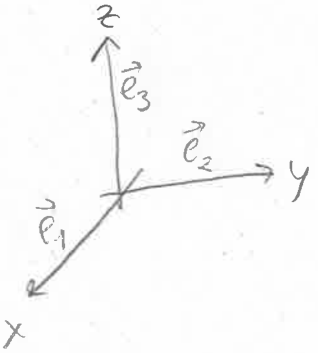
$$\Rightarrow \underline{\delta}\,\phi(\underline{x},\underline{x}'+\underline{\delta}) \simeq \underline{\delta}\,\phi(\underline{x},\underline{x}') + O(\underline{\delta}^2)$$

Therefore, we write, for the i-th component

$$\underbrace{\vec{e}_i \cdot [\hat{\underline{X}}}_{=\hat{X}_i}, \hat{T}(\underline{\delta})] = \vec{e}_i \cdot \underline{\delta} \quad \Leftrightarrow [\hat{X}_i, \hat{T}(\underline{\delta})] = \vec{e}_i \cdot \underline{\delta}$$

If we choose $\underline{\delta} = \epsilon \vec{e}_j$ $\quad (j = 1, 2, 3)$

$$\Rightarrow \quad \underline{\delta} \cdot \vec{e}_i = \epsilon \vec{e}_j \cdot \vec{e}_i = \epsilon \delta_{ij}$$



$$[\hat{X}_i, \hat{T}(\epsilon \vec{e}_j)] = [\hat{X}_i, \hat{I} - i\epsilon \hat{K}_j]$$

$$= -i \cancel{\epsilon} [\hat{X}_i, \hat{K}_j] = \cancel{\epsilon} \delta_{ij}$$

$$\Leftrightarrow \boxed{[\hat{X}_i, \hat{K}_j] = +i\delta_{ij}}$$

We DEFINE the MOMENTUM OPERATOR as the generator of spatial displacement, that is:

$$\hat{\underline{P}} \equiv \frac{1}{\hbar} \hat{\underline{K}} \quad \text{or} \quad \hat{P}_i = \frac{\hat{K}_i}{\hbar}$$

$\hbar$ = reduced Planck constant

Therefore

$$\boxed{[\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}}$$

$\Uparrow$

Fundamental relation in QM!

From $[\hat{T}(\underline{\delta}'), \hat{T}(\underline{\delta}'')] = 0$ it follows that

$$\boxed{[\hat{P}_i, \hat{P}_j] = 0}$$

To find $\hat{T}(\underline{a})$ for a finite displacement $\underline{a}$, note that if

$$\underline{a} = a_1\vec{e}_1 + a_2\vec{e}_2 + a_3\vec{e}_3$$

then

$$\hat{T}(\underline{a}) = \hat{T}(a_1\vec{e}_1 + a_2\vec{e}_2 + a_3\vec{e}_3)$$
$$= \hat{T}(a_1\vec{e}_1)\hat{T}(a_2\vec{e}_2)\hat{T}(a_3\vec{e}_3)$$

So, let us consider only displacement in a fixed direction along the axes:

$$\hat{T}(a_i\vec{e}_i)$$

let $\underline{\epsilon} = \epsilon\vec{e}_i$ with $\epsilon \ll 1$

Then

$$\hat{T}(a\vec{e}_i + \epsilon\vec{e}_i) = \hat{T}(a\vec{e}_i)\hat{T}(\epsilon\vec{e}_i)$$
$$\simeq \hat{T}(a\vec{e}_i)(1 - i\epsilon\hat{K}_i)$$
$$= \hat{T}(a\vec{e}_i) - i\epsilon\hat{T}(a\vec{e}_i)\hat{K}_i$$

Then

$$\frac{d\hat{T}(a\vec{e}_i)}{da} = \lim_{\epsilon \to 0} \frac{\hat{T}((a+\epsilon)\vec{e}_i) - \hat{T}(a\vec{e}_i)}{\epsilon} = -i\hat{T}(a\vec{e}_i)\hat{K}_i$$

Remembering that

$$\frac{d}{dx}\left(e^{-i\lambda x}\right) = -i\lambda e^{-i\lambda x}$$

we find that:

$$\boxed{\hat{T}(a\vec{e}_i) = \exp\left(-i a \hat{K}_i\right)}$$

Therefore, in the general case:

$$\boxed{\hat{T}(\underline{a}) = \exp\left(-\frac{i}{\hbar}\underline{\hat{p}}\cdot\underline{a}\right)}$$

Since $\left(\hat{T}(\epsilon\vec{e}_i)\psi\right)(\underline{x}) = \psi(\underline{x}+\epsilon\vec{e}_i)$

$$\simeq \psi(\underline{x}) + \epsilon\frac{\partial\psi}{\partial x_i}(\underline{x}) + O(\epsilon^2)$$

$$= \left(1 - \epsilon\frac{\partial}{\partial x_i}\right)\psi(\underline{x}) + \dots$$

However,

$$T(\epsilon\vec{e}_i) \simeq \hat{I} - \frac{i}{\hbar}\hat{P}_i\epsilon \Rightarrow \left(T(\epsilon\vec{e}_i)\psi\right)(\underline{x}) \simeq \psi(\underline{x}) - \frac{i}{\hbar}\epsilon(\hat{P}_i\psi)(\underline{x})$$

Therefore, $-\frac{i}{\hbar}\cancel{\epsilon}(\hat{P}_i\psi)(\underline{x}) = -\cancel{\epsilon}\frac{\partial}{\partial x_i}\psi(\underline{x}) \Rightarrow$

$$\Rightarrow \boxed{\hat{P}_i = -i\hbar\frac{\partial}{\partial x_i}}$$

* The momentum operator $\hat{\underline{P}}$ *

The quantum operator associated to the physical observable "linear momentum $\underline{P}$" is

$$\boxed{\hat{\underline{P}} = -i\hbar \vec{\nabla}}$$

We can verify easily that with this $\hat{\underline{P}}$ we have:

$$[\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}$$

Indeed, if $f(\underline{x})$ is a good function, then

$$[\hat{X}_i, \hat{P}_j] f(\underline{x}) = \hat{x}_i(\hat{P}_j f) - \hat{P}_j(\hat{x}_i f)$$

$$= -i\hbar\left[x_i \frac{\partial f}{\partial x_j} - \frac{\partial}{\partial x_j}(x_i f)\right]$$

$$= -i\hbar\left[x_i \frac{\partial f}{\partial x_j} - \underbrace{\frac{\partial x_i}{\partial x_j}}_{=\delta_{ij}} f - x_i \frac{\partial f}{\partial x_j}\right]$$

cancel each other

$$= i\hbar\delta_{ij} f(\underline{x})$$ c.v.d

This operator is Hermitian for functions $\psi(\underline{x}), \varphi(\underline{x})$ that go to zero for $|\underline{x}| \to \infty$:

$$\int \varphi(\hat{P}_i \psi)\, dx_i = -i\hbar \int \varphi \frac{\partial \psi}{\partial x_i} dx_i$$

The rule of integration by part tells us that:

from
$$\frac{d}{dx}(f g) = f\frac{dg}{dx} + \frac{df}{dx} g$$

it follows that:
$$\int_a^b f\frac{dg}{dx}dx = -\int_a^b \frac{df}{dx} g\, dx + \underbrace{fg\Big|_a^b}_{=0 \text{ if } f(a)=f(b)=0}$$

therefore
$$\int \varphi(\hat{P}_i \psi)dx_i = -i\hbar \int \varphi \frac{\partial \psi}{\partial x_i} dx_i$$
$$= i\hbar \int \psi \frac{\partial \varphi}{\partial x_i} dx_i - i\hbar \underbrace{\varphi\psi\Big|_{-\infty}^{\infty}}_{=0}$$
$$= \int \psi (\hat{P}_i^* \varphi) dx_i$$

from the def of Transpose
$$= \int \varphi (\hat{P}_i^\dagger \psi) dx_i$$

So:
$$\int \varphi(\hat{P}_i \psi)dx_i = \int \varphi(\hat{P}_i^\dagger \psi)dx_i \qquad \text{c.v.d}$$

The eigenfunctions $\phi(\underline{x}, \underline{p})$ are, by definition, the solutions of

$$-i\hbar \vec{\nabla} \phi(\underline{x}, \underline{p}) = \underline{p}\, \phi(\underline{x}, \underline{p})$$

This separates in three indep. equations:

$$\phi(\underline{x}, \underline{p}) = \phi(\underline{x}, p_1)\, \phi(\underline{x}, p_2)\, \phi(\underline{x}, p_3)$$

where

$$-i\hbar \frac{\partial \phi(\underline{x}, p_i)}{\partial x_i} = p_i\, \phi(\underline{x}, p_i)$$

The solutions have the form:

$$\phi(\underline{x}, p_i) = \text{constant} \times \exp\left(i \frac{p_i x_i}{\hbar}\right)$$

$$\Rightarrow \quad \boxed{\phi(\underline{x}, \underline{p}) = \text{const.} \exp\left(\frac{i}{\hbar} \underline{p} \cdot \underline{x}\right)}$$

The constant is determined by normalization Eq. (5).

$$\underbrace{\int \phi^*(\underline{x}, \underline{p})\, \phi(\underline{x}, \underline{p}')\, d^3\underline{x}} = \delta(\underline{p}' - \underline{p})$$

$$= |\text{const.}|^2 \int \exp\left[\frac{i}{\hbar}(\underline{p}' - \underline{p}) \cdot \underline{x}\right] d^3x$$

$$= |\text{const.}|^2 (2\pi)^3\, \delta\left(\frac{\underline{p}' - \underline{p}}{\hbar}\right)$$

$$= |\text{const.}|^2 (2\pi\hbar)^3\, \delta(\underline{p}' - \underline{p}) \quad = \delta(\underline{p}' - \underline{p}) \quad \Rightarrow$$

$$\Rightarrow |\text{const.}|^2 = \frac{1}{(2\pi\hbar)^3}$$

We arbitrarily choose const. > 0 $\Rightarrow$

$$\Rightarrow \quad \boxed{\phi(\underline{x}, \underline{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \exp\left(\frac{i}{\hbar} \underline{p} \cdot \underline{x}\right)}$$

According to (4b), we can write the wave function $\psi(\underline{x})$ of the system as an expansion in terms of the functions $\phi(\underline{x}, \underline{p})$:

This stands for a triple integral

$$\psi(\underline{x}) = \int a(\underline{p})\, \phi(\underline{x}, \underline{p})\, d^3p$$

$$= \frac{1}{(2\pi\hbar)^{3/2}} \int a(\underline{p}) \exp\left(\frac{i}{\hbar} \underline{p} \cdot \underline{x}\right) d^3p$$

where, from (4):

$$a(\underline{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\underline{x}) \exp\left(-\frac{i}{\hbar} \underline{p} \cdot \underline{x}\right) d^3x$$

If we make the change of variable $\underline{p} = \hbar \underline{k}$

then $\psi(\underline{x}) = \frac{1}{(2\pi)^{3/2}} \int \left[\hbar^{3/2} a(\hbar \underline{k})\right] \exp(i \underline{k} \cdot \underline{x})\, d^3x$

this coincides with the Fourier transform of $\psi(\underline{x})$ with $\tilde{\psi}(\underline{k}) \equiv \hbar^{3/2} a(\hbar \underline{k})$ <=>

So, we have that:

$a(\underline{p})$ = wave function in representation $\underline{p}$

= FT of $\psi(\underline{x})$

To find the expression of $\hat{\underline{x}}$ in representation $\underline{p}$

we start by writing:

$$\langle \underline{x} \rangle = \int \psi^*(\underline{x})(\hat{\underline{x}}\psi)(\underline{x})\, d^3x$$

$$= \int \psi^*(\underline{x})\, \underline{x}\, \psi(\underline{x})\, d^3x$$

however,

$$\underline{x}\,\psi(\underline{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \int a(\underline{p})\, \underbrace{\underline{x} \exp\left(\frac{i}{\hbar}\underline{p}\cdot\underline{x}\right)}_{= \frac{\hbar}{i}\frac{\partial}{\partial \underline{p}} \exp\left(\frac{i}{\hbar}\underline{p}\cdot\underline{x}\right)} d^3p$$

where $\frac{\partial}{\partial \underline{p}}$ is a short hand for $\left(\frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \frac{\partial}{\partial p_3}\right)$

So $$\underline{x}\,\psi(\underline{x}) = \frac{-i\hbar}{(2\pi\hbar)^{3/2}} \int a(\underline{p}) \frac{\partial}{\partial \underline{p}}\left(e^{\frac{i}{\hbar}\underline{p}\cdot\underline{x}}\right) d^3p$$

integration by parts $$= \frac{-i\hbar}{(2\pi\hbar)^{3/2}} \left\{ \underbrace{a(\underline{p})\, e^{\frac{i}{\hbar}\underline{p}\cdot\underline{x}} \Big|_{-\infty}^{\infty}}_{=0} - \int \frac{\partial a}{\partial \underline{p}}\, e^{\frac{i}{\hbar}\underline{p}\cdot\underline{x}}\, d^3p \right\}$$

$$\underline{x}\,\varphi(\underline{x}) = \frac{i\hbar}{(2\pi\hbar)^{3/2}} \int \frac{\partial a}{\partial \underline{p}} e^{\frac{i}{\hbar}\underline{p}\cdot\underline{x}} d^3p$$

Therefore:

$$\langle \underline{x} \rangle = \frac{i\hbar}{(2\pi\hbar)^{3/2}} \iint \psi^*(\underline{x}) \frac{\partial a}{\partial \underline{p}} \exp\left(\frac{i}{\hbar}\underline{p}\cdot\underline{x}\right) d^3p\, d^3x$$

$$= i\hbar \int \frac{\partial a}{\partial \underline{p}} \underbrace{\left[\frac{1}{(2\pi\hbar)^{3/2}} \int \psi^*(\underline{x}) \exp\left(\frac{i}{\hbar}\underline{p}\cdot\underline{x}\right) d^3x\right]}_{= a^*(\underline{p}) \text{ by def}} d^3p$$

$$= \int a^*(\underline{p}) \left(i\hbar \frac{\partial}{\partial \underline{p}}\right) a(\underline{p})\, d^3p$$

Therefore $\boxed{(\hat{X}\varphi)(\underline{p}) = i\hbar \frac{\partial \varphi}{\partial \underline{p}}}$

The eigenvalues and eigenfunctions are found by solving Eq (12b) p-10:

independent variable

$$\hat{X}(\varphi)(\underline{p}) = \underline{x}\,\varphi(\underline{p}, \underline{x}) \iff i\hbar \frac{\partial \varphi}{\partial \underline{p}} = \underline{x}\,\varphi(\underline{p}, \underline{x})$$

The eigenvalues are independent from the representation

parameter

From page 20 it follows that:

$$\boxed{\varphi(\underline{p}, \underline{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \exp\left(-\frac{i}{\hbar}\underline{p}\cdot\underline{x}\right) = \phi^*(\underline{x}, \underline{p})}$$

c.v.d

* Uncertainty relations *

Let f, g two observables and $\hat{f}$, $\hat{g}$ the corresponding Hermitian operators. Let $\psi(q)$ be the wavefunction of the system.

Define the two new operators $\hat{\Delta f}$ and $\hat{\Delta g}$ defined as:

$$\hat{\Delta f} \equiv \hat{f} - \langle \hat{f} \rangle \quad ; \quad \hat{\Delta g} \equiv \hat{g} - \langle \hat{g} \rangle$$

where, $\langle f \rangle = \int \psi^* (\hat{f}\psi)\, dq \quad , \quad \langle g \rangle = \int \psi^* (\hat{g}\psi)\, dq$

By definition:

$$\langle (\hat{\Delta f})^2 \rangle = \langle (\hat{f} - \langle \hat{f} \rangle)^2 \rangle$$

$$= \langle \hat{f}^2 - 2\langle \hat{f} \rangle \hat{f} + \langle \hat{f} \rangle^2 \rangle$$

From the linearity of the expectation value.

$$= \langle \hat{f}^2 \rangle - 2\langle \hat{f} \rangle \langle \hat{f} \rangle + \langle \hat{f} \rangle^2$$

$$= \langle \hat{f}^2 \rangle - \langle \hat{f} \rangle^2 \equiv$$ VARIANCE of the operator $\hat{f}$

The same relation

$$\langle (\hat{\Delta g})^2 \rangle = \langle \hat{g}^2 \rangle - \langle \hat{g} \rangle^2$$

holds true for $\hat{g}$.

We want to prove that.

$$\boxed{\langle(\hat{\Delta f})^2\rangle\langle(\hat{\Delta g})^2\rangle \geq \frac{1}{4}\left|\langle[\hat{f},\hat{g}]\rangle\right|^2}$$

- Proof

We recall the Schwartz inequality:

If $\psi(q)$, $\phi(q)$ are two wave functions, then

$$\int|\psi|^2 dq \int|\phi|^2 dq' \geq \left|\int\psi^*\phi\, dq\right|^2$$

In fact, if we define

$$\varphi = \psi + \lambda\phi, \quad \text{where } \lambda \in \mathbb{C}$$

then $\int|\varphi|^2 dq \geq 0$

where $|\varphi|^2 = (\psi+\lambda\phi)^*(\psi+\lambda\phi)$

$$= |\psi|^2 + \lambda\psi^*\phi + \lambda^*\phi^*\psi + |\lambda|^2|\phi|^2$$

Therefore

$$\int|\varphi|^2 dq = \int|\psi|^2 dq + \lambda\int\psi^*\phi\, dq + \lambda^*\int\phi^*\psi\, dq + |\lambda|^2\int|\phi|^2 dq \geq 0$$

Since λ is arbitrary, I choose:

$$\lambda = -\frac{\int\phi^*\psi\, dq}{\int|\phi|^2 dq}$$

Using This expression, we get:

$$\int|\varphi|^2 dq = \int|\psi|^2 dq - \frac{\left(\int\phi^*\psi\, dq\right)\left(\int\psi^*\phi\, dq\right)}{\int|\phi|^2 dq} - \frac{\left(\int\phi\psi^* dq\right)\left(\int\phi^*\psi\, dq\right)}{\int|\phi|^2 dq} +$$

$$+ \frac{\left(\int\phi^*\psi\, dq\right)\left(\int\phi\psi^* dq\right)}{\left(\int|\phi|^2 dq\right)^{\cancel{2}}} \cancel{\int|\phi|^2 dq} \geq 0$$

$$= \int|\psi|^2 dq - \frac{\left|\int\phi\psi^* dq\right|^2}{\int|\phi|^2 dq} \geq 0$$

$$\Leftrightarrow \quad \int|\psi|^2 dq \int|\phi|^2 dq \geq \left|\int\phi\psi^* dq\right|^2 \qquad \text{c.v.d}$$

– end of the proof

Now, define $\alpha(q)$ and $\beta(q)$ as:

$$\alpha(q) \equiv (\hat{\Delta f}\psi)(q)$$

$$\beta(q) \equiv (\hat{\Delta g}\psi)(q)$$

Then $$\int|\alpha|^2 dq \int|\beta|^2 dq \geq \left|\int\alpha^*\beta\, dq\right|^2$$

$$\Leftrightarrow \int(\hat{\Delta f}\psi)^*(\hat{\Delta f}\psi)\, dq \int(\hat{\Delta g}\psi)^*(\hat{\Delta g}\psi)\, dq \geq \underbrace{\left|\int(\hat{\Delta f}\psi)^*(\hat{\Delta g}\psi)\, dq\right|^2}_{(1.26)}$$

However

$$\int (\hat{\Delta f}\psi)^*(\hat{\Delta f}\psi)\,dq = \int\left[(\hat{f}^*\psi^*) - \langle\hat{f}\rangle\psi^*\right]\left[(\hat{f}\psi) - \langle\hat{f}\rangle\psi\right]dq$$

$$= \int(\hat{f}^*\psi^*)(\hat{f}\psi) - \langle\hat{f}\rangle\int(\hat{f}^*\psi^*)\psi\,dq$$

$$- \langle\hat{f}\rangle\int\psi^*(\hat{f}\psi)\,dq + \langle\hat{f}\rangle^2\overbrace{\int\psi^*\psi\,dq}^{=1}$$

Remember:

$\int\phi(\hat{f}\psi)dq = \int\psi(\hat{f}^T\phi)dq$

and $(\hat{f}^*)^T = \hat{f}^\dagger = \hat{f}$

$$= \int\psi^*(\hat{f})^2\psi - \langle\hat{f}\rangle\langle\hat{f}\rangle - \langle\hat{f}\rangle\langle\hat{f}\rangle - \langle\hat{f}\rangle^2$$

$$= \int\psi^*(\hat{f}^2 - \langle\hat{f}\rangle^2)\psi\,dq$$

$$= \langle(\hat{\Delta f})^2\rangle$$

The same holds true for $\hat{g}$

To evaluate (1.26), we use again the definition of transposed operator to write

$$\int(\hat{\Delta f}\psi)^*(\hat{\Delta g}\psi)dq = \int\psi^*(\hat{\Delta f}\hat{\Delta g}\psi)\,dq = \langle\hat{\Delta f}\hat{\Delta g}\rangle$$

where we used $\quad \hat{\Delta f} = (\hat{\Delta f})^\dagger$

Now, note that:

$$\hat{\Delta f}\hat{\Delta g} = \frac{1}{2}(\hat{\Delta f}\hat{\Delta g} - \hat{\Delta g}\hat{\Delta f}) + \frac{1}{2}(\hat{\Delta f}\hat{\Delta g} + \hat{\Delta g}\hat{\Delta f})$$

$$\equiv \frac{1}{2}[\hat{\Delta f},\hat{\Delta g}] + \frac{1}{2}\{\hat{\Delta f},\hat{\Delta g}\}$$

curly brackets = symbol of anticommutator: $\{\hat{a},\hat{b}\} = \hat{a}\hat{b} + \hat{b}\hat{a}$

Of course

$$[\Delta\hat{f}, \Delta\hat{g}]^{+} = \Delta\hat{g}^{+}\Delta\hat{f}^{+} - \Delta\hat{f}^{+}\Delta\hat{g}^{+}$$

$$= \Delta\hat{g}\,\Delta\hat{f} - \Delta\hat{f}\,\Delta\hat{g} = -[\Delta\hat{f}, \Delta\hat{g}]$$

and $\{\Delta\hat{f}, \Delta\hat{g}\}^{+} = \{\Delta\hat{f}, \Delta\hat{g}\} \Rightarrow \langle\{\Delta\hat{f}, \Delta\hat{g}\}\rangle \in \mathbb{R}$

The commutator instead is anti-Hermitian, namely

$$\hat{A}^{+} = -\hat{A}$$

For these operators $\langle\hat{A}\rangle_{\psi} = i \times$ (real number)

- Proof

$$\hat{A}^{+} = -\hat{A} \Rightarrow \langle\hat{A}^{+}\rangle = -\langle\hat{A}\rangle$$

but $\langle\hat{A}^{+}\rangle = \int \psi^{*}(A^{+}\psi)\,d\psi = \int \psi(\hat{A}^{*}\psi^{*})\,d\psi$

$$= \left(\int \psi^{*}\hat{A}\psi\,d\psi\right)^{*} = \langle\hat{A}\rangle^{*}$$

therefore

$$\langle\hat{A}^{+}\rangle = -\langle\hat{A}\rangle \Leftrightarrow \langle\hat{A}\rangle^{*} = -\langle\hat{A}\rangle \quad \text{c.v.d}$$

- end of the proof

Then, we can write

$$|\langle\Delta\hat{f}\,\Delta\hat{g}\rangle|^{2} = \Big|\underbrace{\tfrac{1}{2}\langle[\Delta\hat{f}, \Delta\hat{g}]\rangle}_{\text{imaginary number}} + \underbrace{\tfrac{1}{2}\langle\{\Delta\hat{f}, \Delta\hat{g}\}\rangle}_{\text{real number}}\Big|^{2}$$

$$= \frac{1}{4}|\langle[\Delta\hat{f}, \Delta\hat{g}]\rangle|^{2} + \underbrace{\frac{1}{4}|\langle\{\Delta\hat{f}, \Delta\hat{g}\}\rangle|^{2}}_{\geq 0}$$

$$\geq \frac{1}{4}|\langle[\Delta\hat{f}, \Delta\hat{g}]\rangle|^{2}$$

Finally, gathering all the results, we find

$$\boxed{\langle (\hat{\Delta f})^2\rangle \langle (\hat{\Delta g})^2\rangle \geq |\langle \hat{\Delta f}\,\hat{\Delta g}\rangle|^2 \geq \frac{1}{4}|\langle [\hat{\Delta f},\hat{\Delta g}]\rangle|^2}$$

— Example —

Take $\left.\begin{aligned}\hat{f} &= \hat{x}\\ \hat{g} &= \hat{P}_x\end{aligned}\right\}$ — one dimensional

then $[\hat{x},\hat{P}_x] = i\hbar \Rightarrow \langle [\hat{x},\hat{P}_x]\rangle = i\hbar$

$$\Rightarrow \boxed{\langle (\Delta\hat{x})^2\rangle \langle (\Delta\hat{P}_x)^2\rangle \geq \frac{\hbar^2}{4}}$$

← Heisenberg relation!

— HOMEWORK —

Given the wave function:

$$\psi(x) = \frac{1}{\pi^{1/4}\sqrt{\sigma}}\cdot \exp\left[i\frac{P_0 x}{\hbar} - \frac{(x-x_0)^2}{2\sigma^2}\right]$$

calculate: ($\hat{P}$ is a shorthand for $\hat{P}_x$)

a) $\langle \hat{x}\rangle$, $\langle \hat{x}^2\rangle$

b) $\langle \hat{P}\rangle$, $\langle \hat{P}^2\rangle$

c) $\langle (\hat{\Delta x})^2\rangle \langle (\hat{\Delta P})^2\rangle$

d) The wave function in the P_x representation $a(P)$

-HOMEWORK-

Using the commutation relation

$$[\hat{A}_1 \hat{A}_2 \cdots \hat{A}_N, \hat{B}] = [\hat{A}_1, \hat{B}]\hat{A}_2\hat{A}_3 \cdots \hat{A}_N + \hat{A}_1[\hat{A}_2, \hat{B}]\hat{A}_3\hat{A}_4 \cdots \hat{A}_N + \dots + \hat{A}_1\hat{A}_2 \cdots \hat{A}_{N-1}[\hat{A}_N, \hat{B}]$$

demonstrate that

$$[\hat{x}_i, G(\hat{\underline{p}})] = i\hbar \frac{\partial G}{\partial \hat{p}_i}$$

and $$[\hat{p}_i, F(\hat{\underline{x}})] = -i\hbar \frac{\partial F}{\partial \hat{x}_i}$$

where G, F are good functions.

-HOMEWORK-

Consider a signal (electric, electromagnetic, or whatever) that oscillates with angular frequency $\omega_0 = 2\pi\nu_0$ for a time interval Δt:

$$f(t) = \begin{cases} e^{-i\omega_0 t}, & 0 \le t \le \Delta t, \\ 0, & t > \tau \end{cases}$$

Quantify the spread of the frequencies around the central value ω_0 and relate it to the time spread Δt.

– HOMEWORK –

Consider the parity operator $\hat{P}$ defined via:

$$\hat{P}\psi(x) = \psi(-x)$$

Answer the following questions:

a) is $\hat{P}$ Hermitian?

b) is $\hat{P}$ Unitary?

c) what are the eigenvalues?

d) what are the eigenfunctions?