Gaussian Wave Packets

Let us consider an example to illustrate ~~one~~ the formalisms. We look at a Gaussian Wave packet, whose x-space wave fn is given by:

$$\langle x'|\alpha\rangle = \frac{1}{\pi^{1/4}\sqrt{d}} \exp\left[ikx' - \frac{x'^2}{2d^2}\right]$$

- This is a plane wave with wave number k, modulated by a Gaussian profile, centered on the origin. If $|x'| > d$, the prob. amplitude falls of exponentially. The prob. density $|\langle x'|\alpha\rangle|^2$ is a Gaussian with width d.

$$\frac{x'^2}{d^2}$$

Let us compute expectation values of x, x^2, p, p^2:

$$\langle x\rangle = \int_{-\infty}^{\infty} dx' \langle\alpha|x'\rangle x' \langle x'|\alpha\rangle = 0 \quad \text{by symmetry.}$$

$$\langle x^2\rangle = \int_{-\infty}^{\infty} dx' \langle\alpha|x'\rangle x'^2 \langle x'|\alpha\rangle$$

$$= \frac{1}{\sqrt{\pi}\, d}\int_{-\infty}^{\infty} dx'\, x'^2 e^{-x'^2/d^2}$$

$$= \frac{d^2}{2} \quad (\text{Show this!})$$

$$\left[\Gamma(z) = \int_0^{\infty} e^{-t}\, t^{z-1}\, dt\right]$$

$$\therefore \langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2 = \frac{d^2}{2}$$ (dispersion for the position operator).

$$\langle p\rangle = \langle\alpha|p|\alpha\rangle = \int_{-\infty}^{\infty} dx'dx'' \langle\alpha|x'\rangle \langle x'|p|x''\rangle \langle x''|\alpha\rangle$$

$$= \int_{-\infty}^{\infty} dx'dx'' \langle\alpha|x'\rangle \left(-i\hbar\frac{\partial}{\partial x'}\right) \delta(x'-x'') \langle x''|\alpha\rangle$$

$$= \int_{-\infty}^{\infty} dx' \left(\frac{1}{\pi^{1/4}\sqrt{d}}\right)^2 e^{-ikx'-(x'^2/2d^2)} \, -i\hbar\frac{\partial}{\partial x'}\left[e^{ikx'-x'^2/2d^2}\right]$$

$$= \int_{-\infty}^{\infty} dx' \, \frac{1}{\sqrt{\pi}\, d} (\hbar k) \, e^{-x'^2/d^2} = \hbar k$$

$$\langle p^2 \rangle = \frac{\hbar^2}{2d^2} + \hbar^2 k^2 \qquad \left(\text{Use: } \langle x' | p^n | \alpha \rangle = (-i\hbar)^n \frac{\partial^n}{\partial x'^n} \langle x' | \alpha \rangle \right)$$

$$\therefore \langle (\Delta p)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{2d^2}.$$

$$\therefore \langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \frac{\hbar^2}{4}$$

→ We have an equality relation in this case! Gaussian wave packet is often called a <u>Minimum Uncertainty wave packet</u>

We can always obtain a mom-space representation of the Gaussian wave packet:

$$\langle p' | \alpha \rangle = \int dx' \, \langle p' | x' \rangle \langle x' | \alpha \rangle$$

$$= \int dx' \, \frac{1}{\pi^{1/4} \sqrt{d}} \frac{1}{\sqrt{2\pi\hbar}} \, e^{-ip'x'/\hbar} \, e^{(ikx' - x'^2/2d^2)}$$

$$= \frac{1}{\pi^{1/4} \sqrt{d}} \frac{1}{\sqrt{2\pi\hbar}} \int dx' \, e^{-\left[(ip'/\hbar - ik) x' + x'^2/2d^2\right]}$$

$$\left(\frac{ip'}{\hbar} - ik \right) x' + x'^2/2d^2 = \text{Num}$$

$$= 2d^2 \left\{ \left(\frac{ip'}{\hbar} - ik \right) x' + x'^2 \right\}$$

$$= \left[x' + d^2 \left(\frac{ip'}{\hbar} - ik \right) \right]^2 - \left[d^2 \left(\frac{ip'}{\hbar} - ik \right) \right]^2$$

$$\Rightarrow e^{-\left[(ip'/\hbar - ik) x' + x'^2/2d^2\right]} = e^{-\frac{1}{2d^2}\left[(x' + d^2 (\frac{ip'}{\hbar} - ik)) \right]^2} \, e^{-\frac{d^2}{2} \left(\frac{p'}{\hbar} - k \right)^2}$$

$$= e^{-(p'-\hbar k)^2 d^2/2\hbar^2} \int_{-\infty}^{\infty} dx' \, e^{-\frac{1}{2d^2}\left[x' + d^2(ip'/\hbar - k)\right]^2} \frac{1}{\sqrt{2\pi\hbar}\,\pi^{1/4}\sqrt{d}}$$

$$= \sqrt{\frac{d}{\hbar\sqrt{\pi}}}\; e^{-(p'-\hbar k)^2 d^2/2\hbar^2}$$

$$\left(y = \frac{x' + d^2(ip'/\hbar - k)}{\sqrt{2}\, d} \right.$$

$$\Rightarrow dy = \frac{dx'}{\sqrt{2}\, d} \quad \text{or} \quad dx' = \sqrt{2}\, d\,(dy)$$

$$\Rightarrow \int_{-\infty}^{\infty} dy\, e^{-y^2} = \sqrt{\pi} \quad \text{Const. which come out: } \frac{\sqrt{2}\, d\sqrt{d}}{\sqrt{2\pi\hbar}\,\pi^{1/4}\sqrt{d}}$$

Gamma fn. $\longrightarrow$

$$= \sqrt{\frac{d}{\hbar\sqrt{\pi}}}$$

$\therefore$ While the Gaussian wave packet is centered abt '0' in x space, it is centered abt $\hbar k$ in mom. space. The widths are inv. prop. to each other.

If $d \to \infty$ $\quad \langle p'|\alpha\rangle \to \delta(p' - \hbar k)$

while $\quad \langle x'|\alpha\rangle \to e^{ikx}$

if $d \to 0$, $\quad \langle p'|\alpha\rangle = \text{Const.}$

$\quad \langle x'|\alpha\rangle \longrightarrow \delta$ fn.

- If we know x accurately, then information on p is not known and vice versa.

- We know that $\phi_\alpha(p') - \psi_\alpha(x')$ are F.T. pairs. If $\psi_\alpha(x')$ is well localized, then it has a large no. of p' components and vice versa.

Generalization to 3D:

Everything that we have done so far can be generalized to 3 dim:

$$\hat{\vec{x}}\,|\vec{x}'\rangle = \vec{x}'\,|\vec{x}'\rangle$$

and

$$\hat{\vec{p}}\,|\vec{p}'\rangle = \vec{p}'\,|\vec{p}'\rangle$$

$$\langle \vec{x}'|\vec{x}''\rangle = \delta^{(3)}(\vec{x}'-\vec{x}'')$$

$$\langle \vec{p}'|\vec{p}''\rangle = \delta^{(3)}(\vec{p}'-\vec{p}'')$$

where:

$$\delta^{(3)}(\vec{x}'-\vec{x}'') = \delta(x'-x'')\,\delta(y'-y'')\,\delta(z-z'') \quad \text{etc.}$$

Completeness:

$$\int d^3x\,|\vec{x}\rangle\langle\vec{x}| = 1$$

$$\int d^3p\,|\vec{p}\rangle\langle\vec{p}| = 1$$

The rep. of $\hat{\vec{p}}$ in $\{|\vec{x}\rangle\}$ basis:

$$\langle\beta|\vec{p}|\alpha\rangle = \int d^3x'\;\psi^*_\beta(\vec{x}')\,(-i\hbar\vec{\nabla})\,\psi_\alpha(\vec{x}')$$

and

$$\langle\vec{x}'|\vec{p}'\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\,e^{i\vec{p}'\cdot\vec{x}'/\hbar}$$

and finally the wave fns:

$$\psi_\alpha(\vec{x}') = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p'\,e^{i\vec{p}'\cdot\vec{x}'/\hbar}\,\phi_\alpha(\vec{p}')$$

$$\phi_\beta(\vec{p}') = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3x'\,e^{-i\vec{p}'\cdot\vec{x}'/\hbar}\,\psi_\alpha(\vec{x}')$$

Time Evolution:

Time is very different compared to $\vec{x}$, $\vec{p}$. Time is a parameter, while position and momentum are operators. Therefore, time is not an observable. Although it will turn out that we will talk of uncertainty between energy and time, there is no symmetrical treatment of space and time in quantum mechanics (Non-relativistic theory). Symmetrical treatment of space and time, but there even position becomes a parameter!

Let us now talk about time evolution: and in particular time evolution operator. We would like to know what happens to ~~a~~ ~~[illegible]~~ state ket $|\alpha\rangle$ with time. Suppose that at time t_0, the state of a system is represented by $|\alpha\rangle$. At a later time t, the state can nolonger be $|\alpha\rangle$ (except under certain special cases). Let us denote the ket at a later time: $|\alpha, t_0; t\rangle$ $\quad (t > t_0)$ i.e. t is a later time.

Time is a continuous parameter $\Rightarrow$

$$\lim_{t \to t_0} |\alpha, t_0; t\rangle \equiv |\alpha\rangle \quad \text{or} \quad |\alpha, t_0; t_0\rangle \equiv |\alpha, t_0\rangle$$

We need to study:

$$|\alpha, t_0\rangle = |\alpha\rangle \xrightarrow[\text{evolution}]{\text{time}} |\alpha, t_0; t\rangle$$

i.e. we would like to know how the ket $|\alpha\rangle$ changes. Assume (analogous to translation), that the 2 kets are related by an operator:

$$|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0) |\alpha, t_0\rangle$$

What should the properties of $\mathcal{U}(t, t_0)$ be?

- Unitary: $\rightarrow$ required to preserve norm (or prob.) under time evolution.

At time t_0, say $|\alpha, t_0\rangle$ has the following expansion in a basis $\{|a'\rangle\}$ (of some operator $\hat{A}$):

$$|\alpha, t_0\rangle = \sum_{a'}{}' \, c_{a'}(t_0)\, |a'\rangle$$

At a later time:

$$|\alpha, t_0; t\rangle = \sum_{a'}{}' \, c_{a'}(t)\, |a'\rangle$$

In general:

$$|c_{a'}(t_0)| \neq |c_{a'}(t)|$$

(of course there are exceptions that we will get to eventually).

But in order to preserve norm at a later time:

$$\sum_{a'}{}' |c_{a'}(t_0)|^2 = \sum_{a'}{}' |c_{a'}(t)|^2$$

i.e.: $\langle \alpha, t_0 | \alpha, t_0\rangle = 1 = \langle \alpha, t_0; t | \alpha, t_0; t\rangle$

$\Rightarrow$ $\mathcal{U}^{\dagger}(t, t_0)\, \mathcal{U}(t, t_0) = 1$ (fundamental property of $\mathcal{U}$)

- We need:

$$\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1)\, \mathcal{U}(t_1, t_0) \qquad (t_2 > t_1 > t_0)$$

$\rightarrow$ Composition of $\mathcal{U}$. – allows us to take small time steps!

- It is useful to define an infinitesimal time evolution operator:

$$|\alpha, t_0; t_0 + dt\rangle = \mathcal{U}(t_0 + dt, t_0)\, |\alpha, t_0\rangle$$

and we require:

~~Ø~~

$$\lim_{dt \to 0} \mathcal{U}(t_0+dt, t_0) = 1 \quad \text{(identity operator)}.$$

Analogous to the translation case, we set:

$$\mathcal{U}(t_0+dt, t_0) = 1 - i\Omega\, dt$$

where Ω is Hermitian:

i.e. $\Omega^\dagger = \Omega$

- Check that prop of $\mathcal{U}$ are satisfied with this defn.

What should Ω be?

$[\Omega] \sim T^{-1}$ (or frequency). We know:

$$E = \hbar\omega \quad \cancel{\text{now:}}$$

Once again we know from classical mechanics that the Hamiltonian generates time evolution. $\therefore$

$$\Omega = H/\hbar$$

$$\therefore \mathcal{U}(t_0+dt, t_0) = 1 - \frac{iH}{\hbar}dt$$

H: Hamiltonian <u>OPERATOR</u>.

Lesson: Build a Hamiltonian in the same way like you would do in classical mechanics, but promote functions to operators!

<u>The Schrödinger Equation</u>: → Fundamental differential Eqn for the time evolution operator $\mathcal{U}(t, t_0)$.

Using the composition property: setting $t_1 \to t$, $t_2 \to t+dt$

$$\mathcal{U}(t+dt, t_0) = \mathcal{U}(t+dt, t)\,\mathcal{U}(t, t_0) = \left(1 - \frac{iH}{\hbar}dt\right)\mathcal{U}(t, t_0)$$

Case 3: Time dependent Hamiltonian, but $[H(t_1), H(t_2)] \neq 0$

Then the formal solution:

$$\mathcal{U}(t, t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \left[H(t_1) H(t_2) \cdots H(t_n) \right]$$

- Dyson's Series - perturbation exp. of this form in QFT.
- We will prove this later on in the Course.

We will see case 1 examples first and later deal with time dependent scenarios as we progress further.

Energy Eigenkets

In order to know the effect of the time evolution operator on an arbitrary ket $|\alpha\rangle$, we need to know its effect on the base kets.

If A is an operator such that $A|a'\rangle = a'|a'\rangle$ and $[A, H] = 0$, then A and H share the same eigenkets $\{|a'\rangle\}$

$\therefore\ H|a'\rangle = E_{a'}|a'\rangle$

$E_{a'}$ are the eigenvalues of H (energy eigenvalues).

Now:

$$\mathcal{U}(t, t_0)\Big|_{t_0=0} = e^{-iHt/\hbar} = \sum_{a''a'} |a''\rangle\langle a''| e^{-iHt/\hbar} |a'\rangle\langle a'|$$

$$= \sum_{a'} |a'\rangle e^{-iE_{a'}t/\hbar} \langle a'|$$

$\therefore$ if $|\alpha, t_0=0\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha, t_0=0\rangle = \sum_{a'} c_{a'}|a'\rangle$

Then:

$$|\alpha, t_0=0; t\rangle = \mathcal{U}(t, t_0=0)\,|\alpha, t_0=0\rangle$$

$$= e^{-iHt/\hbar}\,|\alpha, t_0=0\rangle$$

$$= \sum_{a'}{}' \langle a'|\alpha\rangle\, e^{-iE_{a'}t/\hbar}$$

Now. $|\alpha, t_0=0; t\rangle = \sum_{a'}{}' C_{a'}(t)\,|a'\rangle$

$\therefore\; C_{a'}(t) = C_{a'}(0)\, e^{-iE_{a'}t/\hbar}$

$\Rightarrow |C_{a'}(t)| = |C_{a'}(0)|$ ($\rightarrow$ This was the special case we had alluded to earlier).

If the initial state $|\alpha, t_0=0\rangle = |a'\rangle$ (eigenstate of A & H).

Then: $|\alpha, t_0; t\rangle = |a'\rangle\, e^{-iE_{a'}t/\hbar}$

$\Rightarrow$ eigenkets have phase modulations alone!

$\therefore$ $\hat{A}$ will have the same eigenkets unchanged by time evolution and in this sense is a const. of motion.

Of course it is possible that more than one operator commutes with H. Then:

$$|K'\rangle = |a', b', c' \ldots\rangle$$

and $$e^{-iHt/\hbar} = \sum_{K'}{}' |K'\rangle\, e^{-iE_{K'}t/\hbar}\,\langle K'|$$

Therefore when the Hamiltonian is time-dependent, the general strategy is to find a maximal set of commuting observables and expand an arbitrary ket in that basis. Once we have the expansion coeffns, we can obtain the state at a later time using the time evolution operator.

Time dependence of expectation values:

Let us assume that $|\alpha, t=0\rangle = |a'\rangle$

where $\hat{A}|a'\rangle = a'|a'\rangle$ and $[A, H] = 0$.

We would like to obtain the ~~eigenkets of $\hat{B}$ where~~ expectation values of $\hat{B}$, where $[B, H] \neq 0$ and $[\hat{A}, \hat{B}] \neq 0$

Now at a later time t:

$|a', t\rangle = \mathcal{U}(t,0)|a'\rangle$

$$\therefore \langle a', t|B|a', t\rangle \equiv \langle B\rangle = \langle a'|e^{-iE_{a'}t/\hbar}\,\hat{B}\,e^{+iE_{a'}t/\hbar}|a'\rangle$$
$$= \langle a'|B|a'\rangle.$$

Therefore the expectation value of an observable taken w.r.t. an energy eigenstate does not change with time. For this reason energy eigenstates are also called stationary states

If $|\alpha, t=0\rangle = \sum'_{a'} c_{a'}(t=0)|a'\rangle$

Then: $$\langle B\rangle = \sum'_{a'a''} c^*_{a''}(t)\, e^{-iE_{a''}t/\hbar}\langle a''|B|a'\rangle c_{a'}(t)\, e^{+iE_{a'}t/\hbar}$$

$$= \sum'_{a'a''} \underbrace{c^*_{a''}(t)c_{a'}(t)\, e^{i(E_{a'}-E_{a''})t/\hbar}}\langle a''|B|a'\rangle$$

Oscillating term with freq: $\omega = \dfrac{E_{a'} - E_{a''}}{\hbar}$

Schrödinger's Wave eqn.

We are now going to obtain the Schrödinger's eqn in the position basis i.e. we will study time evolution of $|\alpha, t_0; t\rangle$ in the $\{|x'\rangle\}$ basis. ie:

$$\psi(\vec{x}', t) = \langle \vec{x}' | \alpha, t_0; t\rangle$$

is the Corresp. wave fn and we will be interested in its time evolution.

$$i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle = H |\alpha, t_0; t\rangle$$

$$\therefore \; i\hbar \frac{\partial}{\partial t} \underbrace{\langle \vec{x}' | \alpha, t_0; t\rangle}_{\Psi(\vec{x}, t)} = \langle x' | H | \alpha, t_0; t\rangle$$

Assume $H = \frac{p^2}{2m} + V(\vec{x})$

$V(\vec{x})$: local operator ~~depends only on~~ $\Rightarrow \langle \vec{x}'' | V(\vec{x}) | \vec{x}'\rangle$
$= V(\vec{x}')\, \delta^{(3)}(\vec{x}' - \vec{x}'')$

We start with the simple form, but $\hat{V}$ could be time dependent, velocity dependent etc.

Now: $\langle \vec{x}' | H | \alpha, t_0; t\rangle = \int d^3x'' \, \langle \vec{x}' | H | \vec{x}''\rangle \, \Psi(\vec{x}'', t)$

$$= \int d^3x'' \left[-\frac{\hbar^2}{2m} \nabla^2_{x''} + V(\vec{x}'') \right] \delta^{(3)}(\vec{x}' - \vec{x}'')\, \Psi(\vec{x}'', t)$$

$$= \left[-\frac{\hbar^2}{2m} \nabla^2_{\vec{x}'} + V(\vec{x}') \right] \Psi(\vec{x}', t)$$

$\therefore$ S. Wave eqn:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{x}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2_{\vec{x}'} \Psi(\vec{x}', t) + V(\vec{x}')\, \Psi(\vec{x}', t) \right]$$

Time - Independent Wave Eqn:

- This the pde satisfied by the energy eigenfunctions.

If $|\alpha, t_0; t\rangle = |a', t_0; t\rangle$

where $|a', t_0; t\rangle$ are the eigenstates of operator $\hat{A}$ such that $[\hat{A}, \hat{H}] = 0$, then:

$$\langle \vec{x}' | a', t_0; t\rangle = \langle \vec{x}' | a'\rangle e^{-iE_{a'}t/\hbar}$$

$$\searrow \langle \vec{x}' | U | \vec{a}', t_0\rangle$$

Plugging this into the TDSE:

$$\langle \vec{x}' | a'\rangle (i\cancel{\hbar}) \left(-\frac{iE_{a'}}{\cancel{\hbar}}\right) = \left[\frac{-\hbar^2}{2m} \nabla^2_{x'} \langle \vec{x}' | a'\rangle + V(\vec{x}') \langle \vec{x}' | a'\rangle \right]$$

or:

$$\underbrace{\left[\frac{-\hbar^2}{2m} \nabla^2_{\vec{x}'} + V(\vec{x}') \right] u_E(\vec{x}') = E_{a'} u_E(\vec{x}')}_{\text{TISE - Time Independent Schrödinger's Eqn.}}$$

$u_E(\vec{x}')$: energy eigenfns.

B.c. $E < \lim_{\vec{x}' \to \infty} V(\vec{x}') \Rightarrow \underbrace{u_E(\vec{x}') \to 0 \text{ as } |\vec{x}'| \to \infty}$

implies that the particle is bound or confined within a finite region of space.

From PDE when the solution is confined to a finite region of space, then it's solution exists only for discrete values of E. It is in this sense, that the TISE yields quantized energy levels.