Time Dependent vs. Independent Wave Equations ①

HW#6 Due by Oct. 25 | Oversea trip for the week of Nov. 13-18 | Oct. 18, 2016

In the last lecture, we started from the Time-Dependent Schrödinger equation and got the Time-Independent (Stationary) Schrödinger Equation for the energy eigenstate. Then, we solved the energy eigenvalue problem for the SHO in 1-dimension using the operator method introducing the annihilation and creation operators,

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) \text{ and } a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right),$$

respectively. From a and $a^\dagger$, the number operator $N = a^\dagger a$ is identified to set the energy base kets

$N|n\rangle = n|n\rangle$, where the physical meaning of n is the number of quanta with the energy $\hbar\omega$ assigned for each quanta. Thus, the energy eigenvalue of SHO can be summarized as

$$H|n\rangle = \left(N + \tfrac{1}{2}\right)\hbar\omega|n\rangle = \underbrace{\left(n + \tfrac{1}{2}\right)\hbar\omega}_{E_n}|n\rangle$$

$E_n = (n+\frac{1}{2})\hbar\omega$ (energy eigenvalue)

$|n\rangle$ (energy eigenstate).

From $\boxed{a|n\rangle = \sqrt{n}\,|n-1\rangle}$, we realized that (2)

n must be non-negative integer.

If we start with a noninteger n, then the sequence of $a^n|n\rangle = \sqrt{n(n-1)(n-2)\cdots 1}\,|0\rangle$ won't terminate leading to eigenkets with a negative value of n.

Note that $\boxed{a|0\rangle = 0}$ must be satisfied. null ket

Using $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$ and $(a^\dagger)^n|0\rangle = \sqrt{n!}\,|n\rangle$

we also found the position representation or spatial wavefunction $\langle x'|n\rangle = \psi_n(x')$ for n'th eigenstate.

Reminder:

$$\boxed{\begin{array}{l} a = \frac{1}{\sqrt{2}x_0}\left(X + \frac{iP}{m\omega}\right) \\ \langle x'|a|0\rangle = 0 \\ \left(x' + x_0^2\frac{d}{dx'}\right)\psi_0(x') = 0 \end{array}}$$

$$\psi_n(x') = \langle x'|n\rangle = \langle x'|\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

$$= \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}x_0}\right)^n\left(x' - x_0^2\frac{d}{dx'}\right)^n\psi_0(x')$$

$$= \frac{1}{\pi^{1/4}\sqrt{x_0}}\frac{1}{\sqrt{2^n n!}}H_n\left(\frac{x'}{x_0}\right)e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2},$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ and $H_n\left(\frac{x'}{x_0}\right)$ is the n'th Hermite polynomial

i.e. $$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) + \frac{1}{2}m\omega^2x^2\psi_n(x) = \left(n+\frac{1}{2}\right)\hbar\omega\,\psi_n(x)}$$

Now, we recall that Heisenberg base kets & bras as well as operators are time-dependent.
How can we understand this from these static energy eigenstates obtained ~~starting~~ from Schrödinger time-dependent state ~~kets~~ $|\alpha, t\rangle$ or $\psi_\alpha(x,t)$? in Schrödinger picture

Recall the relation between Heisenberg and Schrödinger base kets.

Heisenberg base ket

$$|n,t\rangle_H = \underbrace{\mathcal{U}^\dagger(t)}_{e^{\frac{iHt}{\hbar}}}|n\rangle \leftarrow \text{Schrödinger base ket}$$

$$= e^{\frac{iE_n t}{\hbar}}|n\rangle$$

$$i\hbar\frac{\partial}{\partial t}|n,t\rangle_H = -H|n,t\rangle_H$$

$$\uparrow$$

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}^\dagger(t)$$

Closure Relation

$$\sum_n |n,t\rangle_H\, {}_H\langle n,t|$$

$$= \sum_n \mathcal{U}^\dagger(t)|n\rangle\langle n|\mathcal{U}(t)$$

$$= \mathcal{U}^\dagger(t)\underbrace{\left(\sum_n |n\rangle\langle n|\right)}_{I}\mathcal{U}(t)$$

$$= \sum_n |n\rangle\langle n| = I$$

This may be also confirmed by checking

$${}_S\langle\alpha,t|A_S|\alpha,t\rangle_S = {}_H\langle\alpha|A_H(t)|\alpha\rangle_H$$

$$a(t)|n,t\rangle_H = \sqrt{n}\,|n-1,t\rangle_H$$

and

$$a^\dagger(t)|n,t\rangle_H = \sqrt{n+1}\,|n+1,t\rangle_H$$

Note that $A_H(t) = \mathcal{U}^\dagger(t)A_S\mathcal{U}(t)$

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

$$\underbrace{\mathcal{U}^\dagger(t)\,a\,\mathcal{U}(t)}_{a(t)}\underbrace{\mathcal{U}^\dagger(t)|n\rangle}_{|n,t\rangle_H}$$

$$= \sqrt{n}\,\underbrace{\mathcal{U}^\dagger(t)|n-1\rangle}_{|n-1,t\rangle_H}$$

i.e.

$$a(t)|n,t\rangle_H = \sqrt{n}\,|n-1,t\rangle_H$$

In Heisenberg picture, using Heisenberg equation,

$$\frac{da(t)}{dt} = \frac{1}{i\hbar}\Big[a(t),\ \underset{\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)}{\underset{\uparrow}{H}}\Big]$$

Note that Commutation Relations in Schrödinger picture work in Heisenberg picture for all equal time

If, $[A_s, B_s] = C_s$,

then $U^\dagger(t)[A_s, B_s]U(t) = U^\dagger(t) C_s U(t)$

so that $[A_H(t), B_H(t)] = C_H(t)$,

$$= \frac{\omega}{i}\left(a(t)a^\dagger(t)a(t) - a^\dagger(t)a(t)a(t)\right)$$

$$= \frac{\omega}{i}\underbrace{\left[a(t), a^\dagger(t)\right]}_{1} a(t)$$

$$= -i\omega a(t) \quad \text{or} \quad \frac{da(t)}{dt} = -i\omega a(t)$$

Thus, $a(t) = a(0)e^{-i\omega t}$,

and $a^\dagger(t) = a^\dagger(0)e^{+i\omega t}$.

Now, $$a(t)|n,t\rangle_H = a(0)e^{-i\omega t}e^{\frac{i E_n t}{\hbar}}|n\rangle \qquad E_n = \left(n+\tfrac{1}{2}\right)\hbar\omega$$

$$= e^{i\{(n+\frac{1}{2})-1\}\omega t}\underbrace{a(0)|n\rangle}_{\sqrt{n}\,|n-1\rangle}$$

$$= \sqrt{n}\, e^{i\{(n-1)+\frac{1}{2}\}\omega t}|n-1\rangle$$

$$= \sqrt{n}\, e^{\frac{i E_{n-1} t}{\hbar}}|n-1\rangle = \sqrt{n}\,|n-1,t\rangle_H$$ as it must be.

Similarly, $a^\dagger(t)|n,t\rangle_H = \sqrt{n+1}\,|n+1,t\rangle_H$.

Also, note that

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

or

$$a|n\rangle\langle n| = \sqrt{n}\,|n-1\rangle\langle n|$$

or

$$a\underbrace{\sum_n |n\rangle\langle n|}_{I} = \sum_n \sqrt{n}\,|n-1\rangle\langle n|$$

or

$$a = \sum_n \sqrt{n}\,|n-1\rangle\langle n|. \quad \text{and} \quad \underbrace{a(t)}_{\text{Heisenberg}} = \mathcal{U}^\dagger(t)\underset{\substack{\uparrow \\ \text{Schrödinger}}}{a}\,\mathcal{U}(t).$$

Thus, $$a(t) = \sum_n \sqrt{n}\,\underbrace{|n-1,t\rangle_H}_{e^{\frac{iE_{n-1}t}{\hbar}}|n-1\rangle}\;\underbrace{{}_H\langle n,t|}_{e^{-\frac{iE_nt}{\hbar}}\langle n|}$$

$$= \sum_n e^{\frac{i(E_{n-1}-E_n)t}{\hbar}}\sqrt{n}\,|n-1\rangle\langle n|$$

$$= \sum_n \underbrace{e^{\frac{i\left[\{(n-1)+\frac{1}{2}\}\hbar\omega - (n+\frac{1}{2})\hbar\omega\right]t}{\hbar}}}_{e^{-i\omega t}}\;\underbrace{\sqrt{n}\,|n-1\rangle\langle n|}_{a(0)}$$

$$= e^{-i\omega t}\,a(0)$$

Likewise, $a^\dagger(t) = e^{i\omega t}a^\dagger(0)$.

We also confirm that

$$x(t) = \sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger(t) + a(t)\right)$$

$$\begin{array}{cc} a^\dagger(t) & a(t) \\ \uparrow & \uparrow \\ \underbrace{a^\dagger(0)}_{\sqrt{\frac{m\omega}{2\hbar}}\left(x(0) - i\frac{p(0)}{m\omega}\right)} e^{i\omega t} & \underbrace{a(0)}_{\sqrt{\frac{m\omega}{2\hbar}}\left(x(0) + i\frac{p(0)}{m\omega}\right)} e^{-i\omega t} \end{array}$$

$$= x(0)\,\frac{e^{i\omega t}+e^{-i\omega t}}{2} + \frac{p(0)}{m\omega}\,\frac{e^{i\omega t}-e^{-i\omega t}}{2i}$$

$$= x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t \quad \leftarrow$$

Similarly, $p(t) = p(0)\cos\omega t - m\omega\, x(0)\sin\omega t.$

Note that $x(t)$ and $p(t)$ satisfy the Heisenberg eqs.

$$\frac{dx(t)}{dt} = \frac{1}{i\hbar}[x(t), H]$$

and $$\frac{dp(t)}{dt} = \frac{1}{i\hbar}[p(t), H]$$

as we have already shown in Heisenberg eq. lecture.

> Derivation of $x(t)$ using ~~the~~ Baker-Hausdorff Lemma is given in the last lecture note on Oct. 13, 2016.

Note also

$$|\alpha, t\rangle_S = e^{-\frac{iHt}{\hbar}} |\alpha, t=0\rangle_S = e^{-\frac{iHt}{\hbar}} |\alpha\rangle_H$$

and

$$|\alpha\rangle_H = \sum_n |n,t\rangle_H \, {}_H\langle n,t|\alpha\rangle_H$$

$$= \sum_n |n\rangle\langle n|\alpha\rangle_H \quad \text{(absence of time-dependence)}$$

or

$$\sum_n |n,t\rangle_H \, {}_H\langle n,t| = \mathcal{U}^\dagger \underbrace{\sum_n |n\rangle\langle n|}_{I} \, \mathcal{U}(t) = \mathcal{U}^\dagger(t)\mathcal{U}(t) = I.$$

or

$$\boxed{\sum_n |n,t\rangle_H \, {}_H\langle n,t| = \sum_n |n\rangle\langle n|}$$

Going back to the time-dependent wave eq., we have

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{x}', t) = -\frac{\hbar^2}{2m}\vec{\nabla}'^2 \psi(\vec{x}', t) + V(\vec{x}')\psi(\vec{x}', t) \quad \cdots (1)$$

Complex conjugation yields

$$-i\hbar \frac{\partial}{\partial t}\psi^*(\vec{x}', t) = -\frac{\hbar^2}{2m}\vec{\nabla}'^2 \psi^*(\vec{x}', t) + V(\vec{x}')\psi^*(\vec{x}', t) \quad \cdot (2)$$

$\psi^*(\vec{x}', t) \times (1) - \psi(\vec{x}', t) \times (2)$ provides

$$i\hbar \frac{\partial}{\partial t}|\psi(\vec{x}', t)|^2 = -\frac{\hbar^2}{2m}\left(\psi^*(\vec{x}', t)\vec{\nabla}'^2\psi(\vec{x}', t) - \psi(\vec{x}', t)\vec{\nabla}'^2\psi^*(\vec{x}', t)\right)$$

$$\frac{\partial}{\partial t}\left|\psi(\vec{x}',t)\right|^2 + \frac{\hbar}{2mi}\left[\psi^*(\vec{x}',t)\vec{\nabla}'^2\psi(\vec{x}',t) - \psi(\vec{x}',t)\vec{\nabla}'^2\psi^*(\vec{x}',t)\right] = 0$$

Now,
$$\psi^*(\vec{x}',t)\vec{\nabla}'^2\psi(\vec{x}',t) - \psi(\vec{x}',t)\vec{\nabla}'^2\psi^*(\vec{x}',t)$$
$$= \vec{\nabla}'\cdot\left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t) - \psi(\vec{x}',t)\vec{\nabla}'\psi^*(\vec{x}',t)\right]$$

since $\vec{\nabla}'\psi^*\cdot\vec{\nabla}'\psi$ terms cancel each other.

Because
$$\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t) = \mathrm{Re}\left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t)\right] + i\,\mathrm{Im}\left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t)\right]$$

and
$$\psi(\vec{x}',t)\vec{\nabla}'\psi^*(\vec{x}',t) = \left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t)\right]^*$$
$$= \mathrm{Re}\left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t)\right] - i\,\mathrm{Im}\left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t)\right]$$

we get
$$\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t) - \psi(\vec{x}',t)\vec{\nabla}'\psi^*(\vec{x}',t)$$
$$= 2i\,\mathrm{Im}\left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t)\right].$$

Thus, we obtain
$$\frac{\partial}{\partial t}\left|\psi(\vec{x}',t)\right|^2 + \frac{\hbar}{m}\vec{\nabla}'\cdot\mathrm{Im}\left[\psi^*(\vec{x}',t)\vec{\nabla}'\psi(\vec{x}',t)\right] = 0$$

$$\frac{\partial}{\partial t}|\psi(\vec{x}',t)|^2 + \frac{\hbar}{2mi}\left[\psi^*(\vec{x}',t)\,\vec{\nabla}'^2\psi(\vec{x}',t) - \psi(\vec{x}',t)\,\vec{\nabla}'^2\psi^*(\vec{x}',t)\right] = 0$$

$$\vec{\nabla}'\cdot\left[\mathrm{Re}\,\psi^*\vec{\nabla}'\psi + i\,\mathrm{Im}\,\psi^*\vec{\nabla}'\psi\right]$$

$$= \mathrm{Re}\left[(\vec{\nabla}'\psi^*)\cdot(\vec{\nabla}'\psi) + \psi^*\vec{\nabla}'^2\psi\right.$$

$$\vec{\nabla}'\cdot\left[\psi^*\vec{\nabla}'\psi - \psi\vec{\nabla}'\psi^*\right]$$

$$= \cancel{\vec{\nabla}'\psi^*\cdot\vec{\nabla}'\psi} + \psi^*\vec{\nabla}'^2\psi - \cancel{\vec{\nabla}'\psi\cdot\vec{\nabla}'\psi^*} - \psi\vec{\nabla}'^2\psi^*$$

$$= \psi^*\vec{\nabla}'^2\psi - \psi\vec{\nabla}'^2\psi^*$$

$$\psi^*\vec{\nabla}'\psi = \mathrm{Re}\,\psi^*\vec{\nabla}'\psi + i\,\mathrm{Im}\,\psi^*\vec{\nabla}'\psi$$

$$(\psi^*\vec{\nabla}'\psi)^* = \psi\vec{\nabla}'\psi^* = \mathrm{Re}\,\psi\vec{\nabla}'\psi^* + i\,\mathrm{Im}\,\psi\vec{\nabla}'\psi^*$$

$$= \mathrm{Re}\,\psi^*\vec{\nabla}'\psi - i\,\mathrm{Im}\,\psi^*\vec{\nabla}'\psi \quad -$$

$$2i\,\mathrm{Im}\,\psi^*\vec{\nabla}'\psi.$$

We identify

$$|\psi(\vec{x}',t)|^2 = \rho(\vec{x}',t) \quad \text{(matter density)}$$

$$\frac{\hbar}{m}\,\mathrm{Im}\left[\psi^*(\vec{x}',t)\,\vec{\nabla}'\psi(\vec{x}',t)\right] = \vec{j}(\vec{x}',t)$$

(matter current).

Then, what we obtained is

$$\frac{\partial \rho(\vec{x}',t)}{\partial t} + \vec{\nabla}'\cdot\vec{j}(\vec{x}',t) = 0$$

Continuity Eq.

Note that

$$\psi(\vec{x}',t) = \sqrt{\rho(\vec{x}',t)}\, e^{i S(\vec{x}',t)}$$

and $$\vec{j}(\vec{x}',t) = \frac{\rho(\vec{x}',t)\,\vec{\nabla}' S(\vec{x}',t)}{m}$$