General idea of wave-packets from an orthonormal set.

6. At this point, we have discovered almost everything of interest about the time-independent 1D SHO problem -- the energies E_n of Eq. (18), the stationary state eigenfcns $\psi_n(x)$ of Eq. (40), etc. But these eigenstates do have a time-dependence: $\psi_n(x) \rightarrow \psi_n(x,t) = \psi_n(x)\, e^{-(i/\hbar)E_n t}$, satisfying Schrödinger's time-dependent eqtn: $[i\hbar(\partial/\partial t) - \mathcal{H}]\,\psi_n(x,t) = 0$. And superpositions of the $\psi_n(x,t)$ can form localized wave-packets which move in space & time, and which provide global information on how the system behaves. In what follows, we will construct a wave-packet from SHO eigenfcns, and discover some interesting quasi-classical facts.

Recall how wave-packets were constructed for the free-particle case...

$$\left.\begin{array}{l}
\left[(-)\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right]\psi_E(x) = E\psi_E(x) \Rightarrow \begin{smallmatrix}\text{stationary}\\ \text{state solns}\end{smallmatrix} : \psi_E(x) = e^{ikx}, \text{ w/ } k^2 = \frac{2mE}{\hbar^2}. \\
\text{Affix t-dependence}: \psi_E(x) \rightarrow \psi_E(x,t) = \psi_E(x)\, e^{-\frac{i}{\hbar}Et} = e^{i(kx-\omega t)},\ \omega = \frac{\hbar k^2}{2m}. \\
\text{Construct packet}: \Psi(x,t) = \sum_E C_E\, \psi_E(x,t) = (1/\sqrt{2\pi})\int_{-\infty}^{\infty} c(k)\, e^{i(kx-\omega(k)t)}\,dk.
\end{array}\right\} \quad (42)$$

The superposition consts $C_E \leftrightarrow c(k)$ are themselves independent of x & t. From the packet Ψ, as such, we learned important facts such as: $\Delta x \Delta k \sim 1$ for the localization of a free particle of mass m.

We can repeat this procedure for m in external potential $V(x)$. As in (42)...

$$\left.\begin{array}{l}
\left[(-)\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi_E(x) = E\psi_E(x) \Rightarrow \begin{smallmatrix}\text{stationary}\\ \text{state solns}\end{smallmatrix} : \psi_E(x), \text{ presumed known}. \\
\text{Affix t-dependence for state E}: \psi_E(x) \rightarrow \psi_E(x,t) = \psi_E(x)\, e^{-\frac{i}{\hbar}Et}. \\
\text{Construct packet}: \Psi(x,t) = \sum_E C_E\, \psi_E(x)\, e^{-(i/\hbar)Et},\ \{C_E\} \text{ indpt of } x \,\&\, t.
\end{array}\right\} \quad (43)$$

This packet Ψ satisfies: $i\hbar\,\partial\Psi/\partial t = \left[-(\hbar^2/2m)\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi$; easy to show. And the expansion coefficients C_E are also easy if the $\psi_E(x)$ are orthonormal:

Properties of general wave-packet $\Psi(x,t) = \sum_E c_E \psi_E(x) e^{-\frac{i}{\hbar}Et}$.

Assume the $\psi_E(x)$ are orthonormal: $\int \psi_{E'}^*(x)\psi_E(x)\,dx = \delta_{E'E}$.

Note: $\Psi(x,0) = \sum_E c_E \psi_E(x)$, for initial value $(t=0)$.

... operate by $\int dx\, \psi_{E'}^*(x) \cdot$ on this last eq^n, to get...

$$\rightarrow \int \psi_{E'}^*(x)\,\Psi(x,0)\,dx = \sum_E c_E \int \psi_{E'}^*(x)\psi_E(x)\,dx = c_{E'}$$

i.e. // $\boxed{c_E = \int \psi_E^*(x)\,\Psi(x,0)\,dx}$ ✓ E = energy eigenstate involved, $\Psi(x,0)$ = initial packet shape. (44)

So, in this case, the evolution of the packet $\Psi(x,t)$ is fixed by $\Psi(x,0)$.

Now we can normalize Ψ, as...

$$\rightarrow \int \Psi^*(x,t)\Psi(x,t)\,dx = \sum_{E,E'} c_E^* c_{E'} e^{\frac{i}{\hbar}(E-E')t} \underbrace{\int \psi_E^*(x)\psi_{E'}(x)\,dx}_{\delta_{EE'}}$$

$$= \sum_E |c_E|^2 = t\text{-indpt cnst} = 1. \qquad (45)$$

And, finally, we can calculate the average energy of packet Ψ by...

$$\rightarrow \langle E\rangle = \int \Psi^*(x,t)\left\{i\hbar\frac{\partial}{\partial t}\right\}\Psi(x,t)\,dx$$

$$= \sum_{E',E} c_{E'}^* c_E \int \psi_{E'}^*(x)e^{+\frac{i}{\hbar}E't}\left\{i\hbar\frac{\partial}{\partial t}\right\}\psi_E(x)e^{-\frac{i}{\hbar}Et}\,dx$$

$$= \sum_{E',E} c_{E'}^* c_E\, e^{\frac{i}{\hbar}(E'-E)t} \cdot E \underbrace{\int \psi_{E'}^*(x)\psi_E(x)\,dx}_{\delta_{E'E}} = \sum_E E|c_E|^2. \qquad (46)$$

For discrete energies $E \rightarrow E_n$, w/ discrete coefficients c_E (from Eq.(44)), the average energy in the packet (as just calculated) is...

$\boxed{\langle E\rangle = \sum_n E_n |c_n|^2}$ ✓ for discrete E_n & $c_n = \int \psi_n^*(x)\Psi(x,0)\,dx$, specified by some quantum # $n = 0, 1, 2, \ldots$ (47)

Altogether, the generalized wave-packet Ψ, suggested in Eq.(43), is an acceptable solution to $i\hbar\,\partial\Psi/\partial t = \mathcal{H}\Psi$, because: (A) it has calculable expansion coefficients c_E, (B) it is normalizable, (C) it has a calculable avg. energy $\langle E\rangle$.

Wave-packet for the SHO eigenfcns.

7. With the machinery of Eqs. (43)-(47) at our disposal, we construct a wave packet out of the time-dependent SHO eigenfcns, viz...

$$\rightarrow \Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x)\, e^{-\frac{i}{\hbar}E_n t} \quad \int^{w/} \psi_n(x) = \mathcal{N}_n e^{-\frac{1}{2}\xi^2} H_n(\xi),\ E_n = (n+\tfrac{1}{2})\hbar\omega;$$
$$\xi = \alpha x,\ \alpha = \sqrt{\frac{m\omega}{\hbar}},\ \mathcal{N}_n = (\alpha/2^n n!\sqrt{\pi})^{1/2}. \tag{48}$$

This packet contains all possible states of the SHO (state n is present whenever $c_n \neq 0$). We use this Ψ to calculate the SHO average position:

$$\rightarrow \langle x\rangle = \int_{-\infty}^{\infty} x\,|\Psi(x,t)|^2 dx = \sum_{n,k=0}^{\infty} c_n^* c_k\, e^{i(n-k)\omega t} \underbrace{\int_{-\infty}^{\infty} \psi_n^*(x)\, x\, \psi_k(x)\, dx}_{\text{call this } \langle n|x|k\rangle}. \tag{49}$$

Evidently, we need to evaluate the integrals...

$$\rightarrow X_{nk} = \int_{-\infty}^{\infty} \psi_n^*(x)\, x\, \psi_k(x)\, dx = \langle n|x|k\rangle. \tag{50}$$

It is possible to use the generating fcn [$g(s,\xi)$ of Eq. (30)] to find the X_{nk}. We shall use a different method, however, based on the following "well-known" (or easily proven) recurrence relation for the $H_k(\xi)$...

$$\rightarrow H_{k+1}(\xi) - 2\xi H_k(\xi) + 2k H_{k-1}(\xi) = 0. \tag{51}$$

From this, after putting in the $\mathcal{N}$'s of Eq. (48), we find...

$$\rightarrow x\,\psi_k(x) = \frac{1}{\alpha}\sqrt{\frac{k+1}{2}}\,\psi_{k+1}(x) + \frac{1}{\alpha}\sqrt{\frac{k}{2}}\,\psi_{k-1}(x), \quad {}^{w/}\ \underline{\alpha = \sqrt{m\omega/\hbar}};$$

$$\text{So}/\!/ \quad X_{nk} = \frac{1}{\alpha}\sqrt{\frac{k+1}{2}} \underbrace{\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_{k+1}(x)\, dx}_{\delta_{n,k+1},\ \text{by orthogonality};} + \frac{1}{\alpha}\sqrt{\frac{k}{2}} \underbrace{\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_{k-1}(x)\, dx}_{\delta_{n,k-1},\ \text{likewise.}}$$

$$\boxed{\langle n|x|k\rangle = \frac{1}{\alpha}\sqrt{n/2}\,\delta_{n-1,k} + \frac{1}{\alpha}\sqrt{(n+1)/2}\,\delta_{n+1,k}}. \tag{52}$$

Use this result in the expression above, Eq. (49), for the avg. position:

$$\left[\!\!\left[\langle x\rangle = \frac{1}{\alpha}\sum_{n=1}^{\infty}\sqrt{\frac{n}{2}}\, c_n^* c_{n-1}\, e^{+i\omega t} + \frac{1}{\alpha}\sum_{n=0}^{\infty}\sqrt{\frac{n+1}{2}}\, c_n^* c_{n+1}\, e^{-i\omega t}\right.\right. . \tag{53}$$

Classical Motion of the QM SHO.

Combine the terms in $\langle x \rangle$ of Eq.(53) by shifting the summand n, so...

$$\rightarrow \langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} \sum_{n=1}^{\infty} \sqrt{n} \left(c_n^* c_{n-1} e^{+i\omega t} + c_{n-1}^* c_n e^{-i\omega t} \right); \tag{54}$$

... let : $c_n = |c_n| e^{i\phi_n}$, and define : $\Delta\phi_n = \phi_n - \phi_{n-1}$...

$$\text{Soy}\quad \underline{\underline{\langle x \rangle = \sqrt{2/m\omega^2} \underbrace{\sum_{n=0}^{\infty}}_{\text{the } n=0 \text{ term contributes nothing}} \sqrt{n\hbar\omega}\, |c_n c_{n-1}| \cos(\omega t - \Delta\phi_n)}}, \text{ exact QM result.} \tag{55}$$

This expression for $\langle x \rangle$ is still exact. Now assume that the packet Ψ describes m in a relatively high state of the SHO, i.e. $n \to$ large. Then...

$n\hbar\omega \simeq E_n$, and: $c_{n-1} \simeq c_n$. Also: $\Delta\phi_n \to \Delta\phi$ ($\sim$ indpt of n).

$$\text{So}\quad \langle x \rangle \simeq \sqrt{2/m\omega^2} \underbrace{\left(\sum_{n=0}^{\infty} \sqrt{E_n}\, |c_n|^2 \right)} \cos(\omega t - \Delta\phi), \text{ as } n \to \text{large}. \tag{56}$$

Just as : $\langle E \rangle = \sum_{n=0}^{\infty} E_n |c_n|^2$ $\surd$ refer. Eq.(47), put : $\langle \sqrt{E} \rangle = \sum_{n=0}^{\infty} \sqrt{E_n}\, |c_n|^2$;

$$\text{Soy}\quad \underline{\underline{\langle x \rangle \simeq \left\langle \sqrt{2E/m\omega^2} \right\rangle \cos(\omega t - \Delta\phi)}}, \text{ for a "high energy" QM SHO.} \tag{57}$$

This last expression for $\langle x \rangle$ is approximate, but still expected to usable if $E_n = (n+\frac{1}{2})\hbar\omega \simeq n\hbar\omega$ for the principal states contained in Ψ; we need $n \geqslant 10$ for errors in $\langle x \rangle \sim$ few %. We go one step farther...

$$\left[\!\left[\begin{matrix} \text{CLASSICAL SHO} \\ \text{TOTAL ENERGY} \end{matrix} \right\} E = \tfrac{1}{2} m\omega^2 x_0^2, \ \text{w/ } x_0 = \begin{matrix}\text{maximum} \\ \text{displacement}\end{matrix} \Rightarrow \underline{\underline{x_0 = \sqrt{\frac{2E}{m\omega^2}}}}. \tag{58}$$

Then, to within the approx$^{\underline{n}}$s of Eq.(57), the QM SHO has the <u>average</u> motion:

$$\boxed{\langle x \rangle = \langle x_0 \rangle \cos(\omega t - \Delta\phi)}, \tag{59}$$

which -- in an expectation value sense -- is "exactly" the same as the classical motion. Details of the wavepacket have dropped out in Eqs.(56) & (57). The motion in (59) results for <u>any</u> Ψ, so long as $n \to$ large. Correspondence Principle!