

an aside on SHO matrix elements

How to calculate  $\langle n | x^2 | n \rangle$  using explicit wfns.

$$\psi_n(x) = \eta_n H_n(s) e^{-\frac{1}{2}s^2}$$

$$\eta_n = \frac{1}{\sqrt{2^n n!}} \left(\frac{c}{\pi}\right)^{1/4}, \quad c = \frac{(km)}{\hbar}$$

$$s = \sqrt{c} x$$

$$\langle n | x | n \rangle = \eta_n^2 \int_{-\infty}^{\infty} H_n(s) e^{-\frac{1}{2}s^2} \underbrace{x H_n(s) e^{-\frac{1}{2}s^2}}_{\frac{1}{\sqrt{c}} s H_n(s)} dx$$

$$s H_n(s) = \frac{1}{2} H_{n+1}(s) + n H_{n-1}(s)$$

$$= \frac{\eta_n^2}{\sqrt{c}} \int_{-\infty}^{\infty} H_n(s) \left\{ \frac{1}{2} H_{n+1}(s) + n H_{n-1}(s) \right\} e^{-\frac{1}{2}s^2} dx = 0$$

similarly

$$\langle n | x^2 | n \rangle = \eta_n^2 \int_{-\infty}^{\infty} H_n(s) e^{-\frac{1}{2}s^2} \underbrace{x^2 H_n(s) e^{-\frac{1}{2}s^2}}_{\frac{1}{c} s^2 H_n(s)} dx$$

$$s^2 H_n(s) = \frac{1}{2} s H_{n+1} + n s H_{n-1} = \frac{1}{2} \left\{ \frac{1}{2} H_{n+2} + (n+1) H_n \right\} + \frac{1}{2} H_n + (n-1) H_{n-2}$$

$$= \frac{\eta_n^2}{c} \int_{-\infty}^{\infty} H_n \cdot \left\{ \frac{1}{4} H_{n+2} + (n+\frac{1}{2}) H_n + n(n-1) H_{n-2} \right\} e^{-\frac{1}{2}s^2} dx$$

$$= \frac{1}{c} (n+\frac{1}{2}) = \frac{\hbar}{(km)^{1/2}} (n+\frac{1}{2})$$

a.b.  $\langle n | \frac{1}{2} k x^2 | n \rangle = \frac{1}{2} \sqrt{\frac{k}{m}} \hbar (n+\frac{1}{2})$   
 $= \frac{1}{2} (n+\frac{1}{2}) \hbar \omega = \frac{1}{2} E_n$

A neater way of writing this:

$$\begin{aligned}
 x \psi_n &= \frac{\eta_n}{\sqrt{c}} s H_n(s) e^{-\frac{1}{2}s^2} \\
 &= \frac{1}{\sqrt{c}} \eta_n \left\{ \frac{1}{2} H_{n+1} + n H_{n-1} \right\} e^{-\frac{1}{2}s^2} \\
 &= \frac{1}{\sqrt{c}} \left\{ \frac{1}{2} \underbrace{\frac{\eta_n}{\eta_{n+1}} \eta_{n+1} H_{n+1} e^{-\frac{1}{2}s^2}}_{\psi_{n+1}} + n \underbrace{\frac{\eta_n}{\eta_{n-1}} \eta_{n-1} H_{n-1} e^{-\frac{1}{2}s^2}}_{\psi_{n-1}} \right\} \\
 &\quad \underbrace{\frac{1}{\sqrt{2(n+1)}}}_{\text{under } \frac{1}{2}} \quad \underbrace{\frac{1}{\sqrt{2n}}}_{\text{under } n}
 \end{aligned}$$

or

$$x \psi_n = \frac{1}{\sqrt{2c}} \left\{ \sqrt{n+1} \psi_{n+1} + \sqrt{n} \psi_{n-1} \right\}$$

or in Dirac notation

$$x |n\rangle = \frac{1}{\sqrt{2c}} \left\{ \sqrt{n+1} |n+1\rangle + \sqrt{n} |n-1\rangle \right\}$$

then clearly

$$x^2 |n\rangle = \frac{1}{2c} \left\{ \sqrt{(n+1)(n+2)} |n+2\rangle + (2n+1) |n\rangle + \sqrt{n(n-1)} |n-2\rangle \right\}$$

$$\begin{aligned}
 \langle n | x^2 |n\rangle &= \frac{1}{2c} \left\{ \sqrt{\underbrace{n(n+2)}_0} + (2n+1) \underbrace{\langle n | n \rangle}_1 + \sqrt{n(n-1)} \underbrace{\langle n | n-2 \rangle}_0 \right\} \\
 &= \frac{1}{c} \left( n + \frac{1}{2} \right) = \frac{\hbar}{(4m)^{1/2}} \left( n + \frac{1}{2} \right) \checkmark
 \end{aligned}$$

Similarly you can work out "momentum" expected values like

$$\langle n | p_x | n \rangle = -i\hbar \int_{-\infty}^{\infty} \psi_n^* \psi_n' dx$$

using

$$\frac{d}{ds} H_n(s) = 2n H_{n-1}(s)$$

In Dirac's form,

$$\begin{aligned} p_x |n\rangle &\rightarrow -i\hbar \underbrace{\frac{d}{dx}}_{\sqrt{c} \frac{d}{ds}} \eta_n H_n(s) e^{-\frac{1}{2}s^2} \\ &= -i\hbar \eta_n \sqrt{c} \left( \frac{dH_n}{ds} - s H_n \right) e^{-\frac{1}{2}s^2} \\ &= -i\hbar \sqrt{c} \eta_n \left\{ \underbrace{2n H_{n-1}}_{-\frac{1}{2} H_{n+1} - n H_{n-1}} - s H_n \right\} e^{-\frac{1}{2}s^2} \\ &= -i\hbar \sqrt{c} \eta_n \left\{ -\frac{1}{2} H_{n+1} + n H_{n-1} \right\} e^{-\frac{1}{2}s^2} \\ &= -i\hbar \sqrt{c} \left\{ -\frac{1}{2} \frac{\eta_n}{\eta_{n+1}} \psi_{n+1} + n \frac{\eta_n}{\eta_{n-1}} \psi_{n-1} \right\} \\ &= + \frac{i\hbar \sqrt{c}}{\sqrt{2}} \left\{ +\sqrt{n+1} \psi_{n+1} - \sqrt{n} \psi_{n-1} \right\} \end{aligned}$$

$$\therefore p_x |n\rangle = i\hbar \sqrt{\frac{c}{2}} \left\{ \sqrt{n+1} |n+1\rangle - \sqrt{n} |n-1\rangle \right\}$$

so  $\langle n | p_x | n \rangle = 0$

$$p_x^2 |n\rangle = -\frac{\hbar^2 c}{2} \left\{ \sqrt{(n+1)(n+2)} |n+2\rangle - (2n+1) |n\rangle + \sqrt{n(n-1)} |n-2\rangle \right\}$$

$$\langle n | p_x^2 | n \rangle = +\hbar^2 c \left( n + \frac{1}{2} \right) = \hbar \sqrt{km} \left( n + \frac{1}{2} \right)$$

$$\text{n.b. } \langle n | KE | n \rangle = \langle n | \frac{p_x^2}{2m} | n \rangle$$

$$= \frac{1}{2m} \hbar \sqrt{km} \left( n + \frac{1}{2} \right)$$

$$= \frac{1}{2} \hbar \sqrt{\frac{k}{m}} \left( n + \frac{1}{2} \right)$$

$$= \frac{1}{2} \cdot \frac{\left( n + \frac{1}{2} \right) \hbar \omega}{E_n} \quad \checkmark$$