Matrix elements for the harmonic oscillator

Although the operator method for the harmonic oscillator is very elegant, we have so far only rederived results we previously obtained from a direct solution of the Schrödinger's equation. The real advantage of the operator approach is for calculating <u>matrix elements.</u>

From the definitions of the

Creation and annihilation operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i\hat{p}_x}{\sqrt{2m\hbar\omega}}$$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{i\hat{p}_x}{\sqrt{2m\hbar\omega}},$$

it follows that

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

$$\hat{p}_x = i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}^{+} - \hat{a}\right)$$

Thus

$$\hat{x}\,\psi_n = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\psi_{n+1} + \sqrt{n}\,\psi_{n-1}\right).$$

This implies that

$$\langle \psi_{n+1} | \hat{x}\,\psi_n \rangle = \sqrt{\frac{\hbar(n+1)}{2m\omega}}$$ and

$\langle \psi_{n-1} | \hat{x}\, \psi_n \rangle = \sqrt{\frac{\hbar n}{2m\omega}}$, all other matrix elements being zero. Since $\hat{x}$ is a hermitian operator, we write

$$\langle \psi_{n+1} | \hat{x} | \psi_n \rangle \equiv \langle n+1 | \hat{x} | n \rangle = \sqrt{\frac{\hbar(n+1)}{2m\omega}},$$

etc. In particular, $\langle x \rangle_n = \langle n | x | n \rangle = 0$ in an energy eigenstate.

Similarly,

$$\hat{p}_x \psi_n = i\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{n+1}\,\psi_{n+1} - \sqrt{n}\,\psi_{n-1}\right)$$

$$\langle n+1 | \hat{p}_x | n \rangle = i\sqrt{\frac{m\hbar\omega(n+1)}{2}},$$

$$\langle n-1 | \hat{p}_x | n \rangle = -i\sqrt{\frac{m\hbar\omega n}{2}}.$$

All other matrix elements of $\hat{p}_x$ are zero. In particular

$\langle p_x \rangle_n = \langle n | \hat{p}_x | n \rangle = 0$ in an energy eigenstate (this is true for any bound state!)

More complex operators

$$\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a}^+ + \hat{a})(\hat{a}^+ + \hat{a})$$

$$= \frac{\hbar}{2m\omega}\left((\hat{a}^+)^2 + \hat{a}^2 + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+\right)$$

$$= \frac{\hbar}{2m\omega}\left((\hat{a}^+)^2 + \hat{a}^2 + 2\hat{a}^+\hat{a} + \underline{1}\right)$$

$$\langle n | \hat{x}^2 | n \rangle = \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)$$

show steps

$$\hat{p}^2 = -\frac{m\hbar\omega}{2}(\hat{a}^+ - \hat{a})(\hat{a}^+ - \hat{a})$$

$$= -\frac{m\hbar\omega}{2}\left((\hat{a}^+)^2 + (\hat{a})^2 - \hat{a}^+\hat{a} - \hat{a}\hat{a}^+\right)$$

$$= m\hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right) - \frac{m\hbar\omega}{2}\left((\hat{a}^+)^2 + \hat{a}^2\right)$$

$$\langle n|\hat{p}^2|n\rangle = m\hbar\omega\left(n + \frac{1}{2}\right)$$

$$\langle\hat{T}\rangle = \langle n|\frac{\hat{p}^2}{2m}|n\rangle = \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right)$$

$$\langle\hat{V}\rangle = \langle n|\frac{m\omega^2\hat{x}^2}{2}|n\rangle = \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right)$$

$$\langle\hat{T}\rangle = \langle\hat{V}\rangle = \frac{\langle\hat{H}\rangle}{2}.$$

This is the virial theorem for a harmonic potential. In general, the virial theorem states

$$2\langle \hat{T} \rangle = \alpha \langle \hat{V} \rangle,$$

for $V(x) \propto x^{\alpha}$.

Of course, all of these matrix elements could also be calculated using the harmonic oscillator wavefunctions $\psi_n(x)$. For example,

$$\langle n | X^2 | n \rangle = \int_{-\infty}^{\infty} dx \, \psi_n^*(x) \, x^2 \, \psi_n(x)$$

$$= \frac{\sqrt{m\omega/\pi\hbar}}{2^n n!} \int_{-\infty}^{\infty} dx \, H_n^2\left(\sqrt{\frac{m\omega}{\hbar}} x\right) e^{-\frac{m\omega x^2}{\hbar}} x^2 .$$

However, most consider the operator method much simpler for such calculations!

<u>Comments</u> Creation and annihilation operators are very useful in many-body

physics and quantum field theory. The excitations of systems of many interacting particles can often be described as coupled harmonic oscillators, and creation and annihilation operators can be introduced for each normal mode of the system. For example, the elementary quanta of vibration in solids are called phonons. The elementary magnetic excitations in a magnetic solid are called magnons. Both types of excitations can be described via operators with the same algebra as the harmonic oscillator

$$[\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha\beta},$$

where α, β refer to the various normal modes.

A similar algebra holds for photons, the quanta of the electromagnetic field.

$$\hat{H} = \sum_\alpha \hbar\omega_\alpha (a_\alpha^\dagger a_\alpha + \tfrac{1}{2})$$