HARMONIC OSCILLATOR - ZERO-POINT ENERGY FROM UNCERTAINTY PRINCIPLE

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3.

There is a nice result derived in Shankar's section 7.3 in which he shows that we can actually derive the ground state energy and wave function for the harmonic oscillator from the uncertainty principle. Classically, the energy of a harmonic oscillator is

$$H=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2 \tag{1}$$

where both p and x are continuous variables that can, in principle, take on any values. Thus classically it is possible for an oscillator to have $x=p=0$ giving a ground state with zero energy. In quantum mechanics, because X and P don't commute, the position and momentum cannot both have precise values, which means that the ground state must have an energy greater than zero. This so-called *zero-point energy* is (as found by Solving Schrödinger's equation)

$$E_0=\frac{\hbar\omega}{2} \tag{2}$$

To derive this without needing to solve Schrödinger's equation, we first recall that a state in which the position-momentum uncertainty is a minimum must be a gaussian of form

$$\Psi(x)=Ae^{-a(x-\langle x\rangle)^2/2\hbar}e^{i\langle p\rangle x/\hbar} \tag{3}$$

where a is a positive real constant, A is the normalization constant, $\langle x\rangle$ is the mean position and $\langle p\rangle$ is the mean momentum. For a harmonic oscillator centred at $x=0$, we have that both $\langle x\rangle=\langle p\rangle=0$, so we know that the ground state wave function has the form

$$\psi(x)=Ae^{-ax^2/2\hbar} \tag{4}$$

To normalize this we require (assuming A is real)

$$\int_{-\infty}^{\infty}\psi^2(x)\,dx=1 \tag{5}$$

Using the standard result for a gaussian integral (see Appendix 2 in Shankar or use Google)

$$\int_{-\infty}^{\infty}\psi^{2}(x)\,dx = A^{2}\int_{-\infty}^{\infty}e^{-ax^{2}/\hbar}dx \tag{6}$$

$$= A^{2}\sqrt{\frac{\pi\hbar}{a}} \tag{7}$$

Therefore

$$A=\left(\frac{a}{\pi\hbar}\right)^{1/4} \tag{8}$$

We need to find a such that $\Delta X\Delta P$ is minimized. The harmonic oscillator hamiltonian is

$$H=\frac{P^{2}}{2m}+\frac{1}{2}m\omega^{2}X^{2} \tag{9}$$

Since $\langle X\rangle=\langle P\rangle=0$, the uncertainties become

$$(\Delta X)^{2} = \left\langle X^{2}\right\rangle-\langle X\rangle^{2}=\left\langle X^{2}\right\rangle \tag{10}$$

$$(\Delta P)^{2} = \left\langle P^{2}\right\rangle-\langle P\rangle^{2}=\left\langle P^{2}\right\rangle \tag{11}$$

Averaging 9 we get

$$\langle H\rangle = \frac{\left\langle P^{2}\right\rangle}{2m}+\frac{1}{2}m\omega^{2}\left\langle X^{2}\right\rangle \tag{12}$$

$$= \frac{(\Delta P)^{2}}{2m}+\frac{1}{2}m\omega^{2}(\Delta X)^{2} \tag{13}$$

At minimum uncertainty

$$\Delta X\Delta P=\frac{\hbar}{2} \tag{14}$$

so we have

$$\Delta P=\frac{\hbar}{2\Delta X} \tag{15}$$

$$\langle H\rangle=\frac{\hbar^{2}}{8m(\Delta X)^{2}}+\frac{1}{2}m\omega^{2}(\Delta X)^{2} \tag{16}$$

The minimum energy can now be found by finding the value of $(\Delta X)^2$ that minimizes this function. Treating $(\Delta X)^2$ (not just ΔX) as the independent variable, we have

$$\frac{\partial \langle H \rangle}{\partial (\Delta X)^2} = -\frac{\hbar^2}{8m\left[(\Delta X)^2\right]^2} + \frac{1}{2}m\omega^2 \tag{17}$$

$$= -\frac{\hbar^2}{8m(\Delta X)^4} + \frac{1}{2}m\omega^2 = 0 \tag{18}$$

$$(\Delta X)^2 = \frac{\hbar}{2m\omega} \tag{19}$$

This gives a minimum value for the mean energy of

$$\langle H \rangle_{min} = \frac{\hbar\omega}{2} \tag{20}$$

To complete the derivation, we need to find the gaussian 4 that gives the correct value 19 for $(\Delta X)^2$. That is, we need to find a such that

$$(\Delta X)^2 = \langle X^2 \rangle = \frac{\hbar}{2m\omega} \tag{21}$$

This requires doing another gaussian integral:

$$\langle X^2 \rangle = \int_{-\infty}^{\infty} x^2 \psi^2(x)\, dx \tag{22}$$

$$= \sqrt{\frac{a}{\pi\hbar}} \int_{-\infty}^{\infty} x^2 e^{-ax^2/\hbar} dx \tag{23}$$

$$= \sqrt{\frac{a}{\pi\hbar}} \sqrt{\frac{\pi\hbar}{a}} \frac{h}{2a} \tag{24}$$

$$= \frac{\hbar}{2a} \tag{25}$$

We therefore get

$$\frac{\hbar}{2a} = \frac{\hbar}{2m\omega} \tag{26}$$

$$a = m\omega \tag{27}$$

which gives a normalized minimum energy wave function

$$\psi_{min}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \tag{28}$$

This is the lowest possible value for the energy, but is it actually the ground state energy? What we have shown so far is that

$$\langle\psi_{min}|H|\psi_{min}\rangle \le \langle\psi_0|H|\psi_0\rangle = E_0 \tag{29}$$

where $|\psi_0\rangle$ is the ground state energy. However, we can invoke the variational principle which states that if ψ is any normalized function, then the ground state energy E_0 of any hamiltonian H satisfies

$$E_0 \le \langle\psi|H|\psi\rangle \tag{30}$$

Using $\psi = \psi_{min}$ we therefore have

$$E_0 \le \langle\psi_{min}|H|\psi_{min}\rangle \tag{31}$$

Combining 29 and 31 we have

$$\langle\psi_{min}|H|\psi_{min}\rangle \le E_0 \le \langle\psi_{min}|H|\psi_{min}\rangle \tag{32}$$

which means that

$$E_0 = \langle\psi_{min}|H|\psi_{min}\rangle \tag{33}$$

and therefore that $|\psi_0\rangle = |\psi_{min}\rangle$, that is, 28 is actually the ground state wave function.

Although this clever little derivation gives us the ground state energy and wave function, it doesn't say anything about the higher energy states, or tell us that they are all equally spaced with a spacing of $\hbar\omega$. Nevertheless, it's a pleasant exercise.