Spring 1999 #8

A particle moves in the potential $V(x) = \begin{cases} \infty & x \le 0 \\ \frac{1}{2}m\omega^2 x^2 & x \ge 0 \end{cases}$

a) Estimate the energy using the variational method with the trial wave function $\psi(x) = \begin{cases} 0 & x \le 0 \\ Nxe^{-\mu x} & x \ge 0 \end{cases}$

Start by finding 'N' using the normalization condition and the hint

$$\int_0^\infty y^n e^{-ay}\,dy = \frac{n!}{a^{n+1}}$$

for the trial wave function

$$\langle\psi|\psi\rangle = \int_0^\infty N^2 x^2 e^{-2\mu x}\,dx = 1$$

$$\frac{N^2(2!)}{(2\mu)^3} = 1 \quad \Rightarrow \quad N = \frac{(2\mu)^{3/2}}{\sqrt{2}} = 2\mu^{3/2}$$

the Hamiltonian for the particle is: $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ (x
we don't need to be concerned with H for $x < 0$ since we know $\psi = 0$ there

Next, calculate $\langle\psi|H|\psi\rangle = \frac{1}{2m}\langle\psi|p^2|\psi\rangle + \frac{1}{2}m\omega^2\langle\psi|x^2|\psi\rangle$

$$\frac{1}{2m}\langle\psi|p^2|\psi\rangle = \frac{-\hbar^2}{2m}\int_0^\infty 4\mu^3 xe^{-\mu x}\left[\left(\frac{d^2}{dx^2}\right)xe^{-\mu x}\right]dx$$

$$= \frac{-2\hbar^2}{m}\mu^3\int_0^\infty xe^{-\mu x}\left(\frac{d}{dx}\right)\left(e^{-\mu x} - \mu xe^{-\mu x}\right)dx$$

$$= \frac{-2\hbar^2\mu^3}{m}\int_0^\infty xe^{-\mu x}\left(-\mu e^{-\mu x} - \mu\left(e^{-\mu x} - \mu xe^{-\mu x}\right)\right)dx$$

$$= \frac{-2\hbar^2\mu^3}{m}\int_0^\infty\left(-\mu xe^{-2\mu x} - \mu xe^{-2\mu x} + \mu^2 x^2 e^{-2\mu x}\right)dx$$

$$= \frac{-2\hbar^2\mu^3}{m}\left[(-2\mu)\frac{1!}{(2\mu)^2} + \mu^2\frac{2!}{(2\mu)^3}\right]$$

$\Rightarrow$

$$\frac{1}{2m}\langle\psi|p^2|\psi\rangle = -\frac{2\hbar^2\mu^3}{m}\left(-\frac{1}{2\mu}+\frac{1}{4\mu}\right)$$

$$= -\frac{2\hbar^2\mu^3}{m}\left(\frac{-1}{4\mu}\right) = \boxed{\frac{\hbar^2\mu^2}{2m} = \langle\psi|p^2|\psi\rangle\frac{1}{2m}}$$

$$\frac{1}{2}m\omega^2\langle\psi|x^2|\psi\rangle = \frac{1}{2}m\omega^2\int_0^\infty 4\mu^3 x^4 e^{-2\mu x}\,dx$$

$$= 2m\omega^2\mu^3\frac{4!}{(2\mu)^5} = \frac{48m\omega^2\mu^3}{32\mu^5} = \boxed{\frac{3m\omega^2}{2\mu^2}}$$

Thus $\langle\psi|H|\psi\rangle = \frac{1}{2}\left(\frac{\hbar^2}{m}\mu^2 + 3m\omega^2\mu^{-2}\right)$

Next find μ to minimize $\langle H\rangle$

$$\frac{d}{d\mu}\left(\frac{\hbar^2}{m}\mu^2 + 3m\omega^2\mu^{-2}\right) = \left(\frac{2\hbar^2}{m}\mu - 6m\omega^2\mu^{-3}\right) = 0$$

$$\frac{2\hbar^2\mu^4}{m} - 6m\omega^2 = 0$$

$$\mu^4 = \frac{6m^2\omega^2}{2\hbar^2} \Rightarrow \mu^2 = \sqrt{3}\,\frac{m\omega}{\hbar}$$

plugging in μ^2 yields

$$\langle H\rangle = \frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\sqrt{3} + \frac{3m\omega^2\hbar}{2m\omega\sqrt{3}} = \boxed{\sqrt{3}\,\hbar\omega = \text{estimated energy}}$$

b) the physical situation corresponds to the odd states of the SHO

$$\left((2n+1)+\frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, 3$$

the energy of the ground state is thus

$$\boxed{E_{ground} = \frac{3}{2}\hbar\omega}$$