Hirophysics.com

The variational method

For 1-dimensional S.H.O., using this traial function,

$$\psi(x,\alpha) = Ce^{-\alpha x^2} \quad (\alpha > 0),$$

find the ground state.

---

① Find the normalized coefficient C.

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

$$\therefore \ C^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = C^2 \sqrt{\frac{\pi}{2\alpha}} = 1 \qquad \left(\because \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \right)$$

Therefore, $C = \left(\frac{2\alpha}{\pi}\right)^{1/4}$

② Calculate the average value for the hamiltonian.

$$I(\alpha) = \int_{-\infty}^{\infty} \psi^* H \psi \, dx = \left(\frac{2\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} e^{-\alpha x^2} \left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right) e^{-\alpha x^2} dx$$

$$= \left(\frac{2\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} e^{-\alpha x^2} \left\{ \frac{-\hbar^2}{2m} \left(-2\alpha e^{-\alpha x^2} + 4\alpha^2 x^2 e^{-\alpha x^2}\right) + \frac{1}{2} m\omega^2 x^2 e^{-\alpha x^2} \right\} dx$$

$$= \left(\frac{2\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} \left[\frac{\hbar^2}{m} \alpha e^{-2\alpha x^2} - \frac{2\hbar^2}{m} \alpha^2 x^2 e^{-2\alpha x^2} + \frac{1}{2} m\omega^2 x^2 e^{-2\alpha x^2} \right] dx$$

$$= \left(\frac{2\alpha}{\pi}\right)^{1/2} \left[\frac{\hbar^2}{m} \alpha \sqrt{\frac{\pi}{2\alpha}} - \frac{2\hbar^2\alpha^2}{m} \frac{1}{4\alpha} \sqrt{\frac{\pi}{2\alpha}} + \frac{m\omega^2}{2} \frac{1}{4\alpha} \sqrt{\frac{\pi}{2\alpha}} \right]$$

$$\boxed{\text{Because} \quad \int_{-\infty}^{\infty} x^p e^{-ax^q} dx = \frac{2}{q a^{(p+1)/q}} \Gamma\left(\frac{p+1}{q}\right) \ ; \qquad \Gamma(x+1) = x\Gamma(x)}$$

$$= \frac{\hbar^2\alpha}{m} - \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}$$

$$= \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}$$

③ Find α to make $I(\alpha)$ minimum.

The condition is $\frac{dI(\alpha)}{d\alpha} = 0$.

$$\frac{d}{d\alpha}\left(\frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}\right) = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2}$$

$$\frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha_0^2} = 0$$

$$\frac{\hbar^2}{2m} = \frac{m\omega^2}{8\alpha_0^2}$$

$$\alpha_0^2 = \frac{2m^2\omega^2}{8\hbar^2}$$

$$\alpha_0 = \frac{1}{2}\sqrt{\frac{m^2\omega^2}{\hbar}} = \frac{m\omega}{2\hbar}$$

④ Plug α_0 into $I(\alpha)$ in order to get E_0 (ground state).

$$E_0 = I(\alpha_0) = \frac{\hbar^2\alpha_0}{2m} + \frac{m\omega^2}{8\alpha_0}$$

$$= \frac{\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{m\omega^2}{8}\frac{2\hbar}{m\omega}$$

$$= \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4}$$

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

⑤ Also determine the eigenfunction.

The trial function was $\psi(x,\alpha) = Ce^{-\alpha x^2}$,

So just plug C and α_0 into there.

$$\psi_0(x,\alpha_0) = \left(\frac{2\alpha_0}{\pi}\right)^{1/4} e^{-\alpha_0 x^2}$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$