

Quantum Mechanics 2

Robert C. Roleda
Physics Department

Variational Method
Harmonic Oscillator



De La Salle University



Harmonic Oscillator

Let us use the variational method to make an approximation of the ground state energy of a harmonic oscillator

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$$

The boundary condition in this case is that the wave function must vanish at $\pm\infty$. One such function is

$$\tilde{\psi} = e^{-\alpha x^2}$$

With this,

$$\langle \tilde{\psi} | \tilde{\psi} \rangle = \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = \sqrt{\frac{\pi}{2\alpha}}$$



Harmonic Oscillator

Now

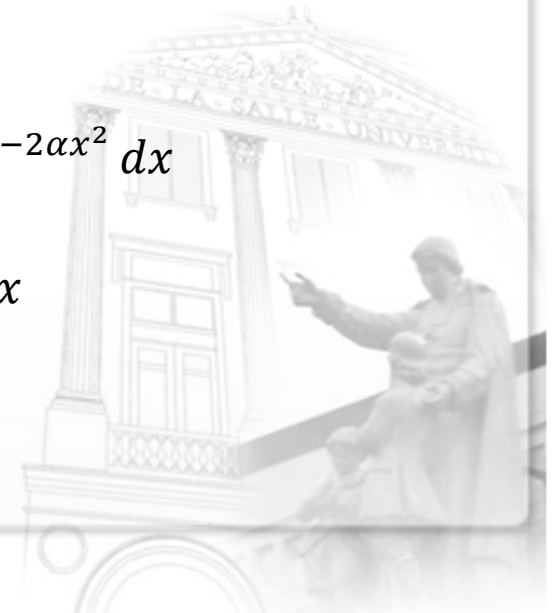
$$\frac{d^2 e^{-\alpha x^2}}{dx^2} = \frac{d}{dx} (-2\alpha x e^{-\alpha x^2}) = -2\alpha e^{-\alpha x^2} + (-2\alpha x)^2 e^{-\alpha x^2}$$

Hence

$$H\tilde{\psi} = -\frac{\hbar^2}{2m} \frac{d^2 e^{-\alpha x^2}}{dx^2} + \frac{1}{2} m\omega^2 x^2 e^{-\alpha x^2} = \left[\frac{\hbar^2 \alpha}{m} - \frac{2\hbar^2 \alpha^2}{m} x^2 + \frac{1}{2} m\omega^2 x^2 \right] e^{-\alpha x^2}$$

Thus,

$$\begin{aligned} \langle \tilde{\psi} | H | \tilde{\psi} \rangle &= \int_{-\infty}^{\infty} \left[\frac{\hbar^2 \alpha}{m} - \frac{2\hbar^2 \alpha^2}{m} x^2 + \frac{1}{2} m\omega^2 x^2 \right] e^{-2\alpha x^2} dx \\ &= 2 \int_0^{\infty} \left[\frac{\hbar^2 \alpha}{m} + \left(\frac{1}{2} m\omega^2 - \frac{2\hbar^2 \alpha^2}{m} \right) x^2 \right] e^{-2\alpha x^2} dx \end{aligned}$$



Harmonic Oscillator

The first term is

$$2 \int_0^{\infty} \frac{\hbar^2 \alpha}{m} e^{-2\alpha x^2} dx = \frac{\hbar^2 \alpha}{m} \sqrt{\frac{\pi}{2\alpha}}$$

The second term may be evaluated using Gamma functions

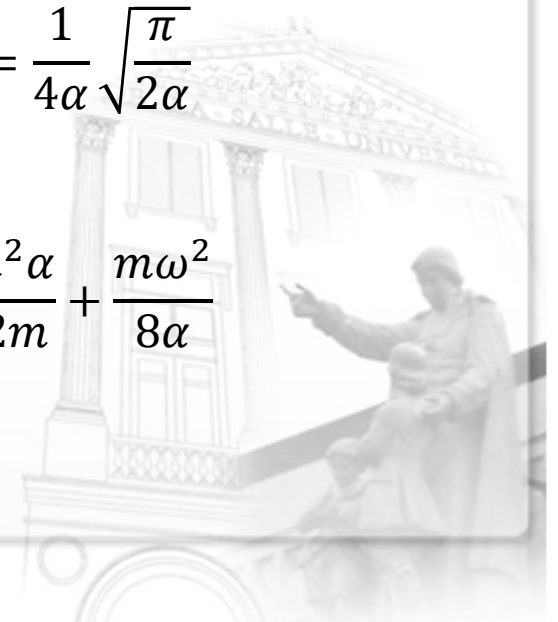
$$\Gamma(z) = 2 \int_0^{\infty} u^{2z-1} e^{-u^2} du$$

So

$$2 \int_0^{\infty} x^2 e^{-2\alpha x^2} dx = \frac{\Gamma(3/2)}{(2\alpha)^{3/2}} = \frac{1}{(2\alpha)^{3/2}} \frac{\Gamma(1/2)}{2} = \frac{1}{4\alpha} \sqrt{\frac{\pi}{2\alpha}}$$

and

$$\bar{H} = \frac{\langle \tilde{\psi} | H | \tilde{\psi} \rangle}{\langle \tilde{\psi} | \tilde{\psi} \rangle} = \frac{\hbar^2 \alpha}{m} + \left(\frac{1}{2} m \omega^2 - \frac{2\hbar^2 \alpha^2}{m} \right) \frac{1}{4\alpha} = \frac{\hbar^2 \alpha}{2m} + \frac{m\omega^2}{8\alpha}$$



Harmonic Oscillator

To optimize, we set

$$\frac{\partial \bar{H}}{\partial \alpha} = 0$$

This yields

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

or

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

This gives

$$\bar{H} = \frac{\hbar^2 \alpha}{2m} + \frac{m\omega^2}{8\alpha} = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

which is the exact value of the ground state.

