

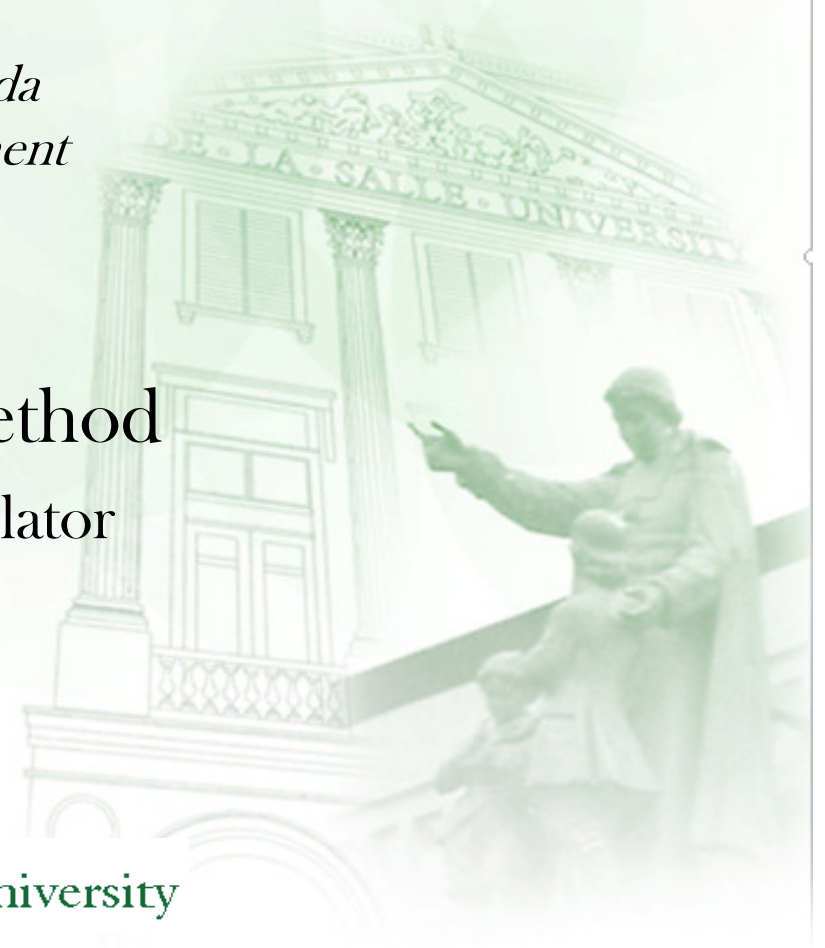
Quantum Mechanics 2

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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

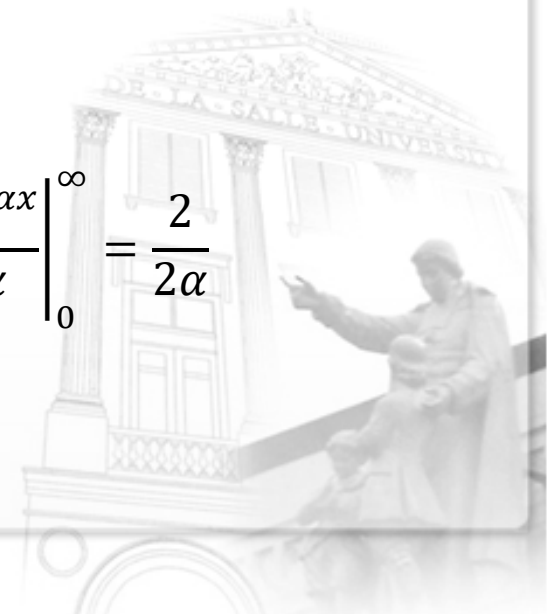
$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$$

The important thing to remember in selecting a trial function is that it must satisfy the boundary conditions of the system. In this case, the boundary condition is that the wave function must vanish at $\pm\infty$. One such function is

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

With this,

$$\langle \tilde{\psi} | \tilde{\psi} \rangle = \int_{-\infty}^{\infty} e^{-2\alpha|x|} dx = 2 \int_0^{\infty} e^{-2\alpha x} dx = -2 \frac{e^{-2\alpha x}}{2\alpha} \Big|_0^{\infty} = \frac{2}{2\alpha}$$



Harmonic Oscillator

For $x < 0$, $x = -|x|$

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

For $x > 0$, $x = |x|$

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

Thus,

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



Harmonic Oscillator

The first term is

$$-\frac{\hbar^2 \alpha^2}{m} \int_0^\infty e^{-2\alpha x} dx = -\frac{\hbar^2 \alpha^2}{m} \frac{1}{2\alpha}$$

The second term may be evaluated using Gamma functions

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt$$

So

$$m\omega^2 \int_0^\infty x^2 e^{-2\alpha x} dx = \frac{m\omega^2}{(2\alpha)^3} \Gamma(3) = \frac{m\omega^2}{(2\alpha)^3} 2!$$

and

$$\bar{H} = \frac{\langle \tilde{\psi} | H | \tilde{\psi} \rangle}{\langle \tilde{\psi} | \tilde{\psi} \rangle} = -\frac{\hbar^2 \alpha^2}{2m} + \frac{m\omega^2}{4\alpha^2}$$



Harmonic Oscillator

To optimize, we set

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

This yields

$$\begin{aligned} -\frac{\hbar^2 \alpha}{m} - \frac{m\omega^2}{2\alpha^3} &= 0 \\ \alpha^4 &= -\frac{m^2 \omega^2}{2\hbar^2} \\ \alpha^2 &= \pm i \frac{m\omega}{\sqrt{2}\hbar} \end{aligned}$$

This however gives

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

This shows that $\tilde{\psi} = e^{-\alpha|x|}$ is not a tenable trial function.

