

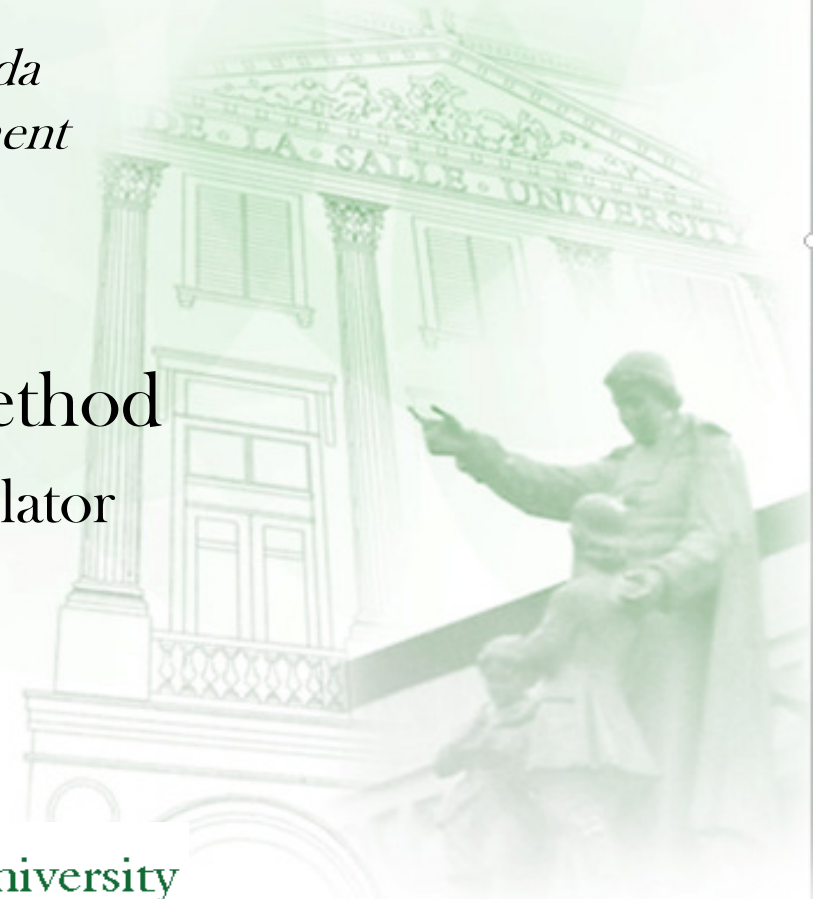
# Quantum Mechanics 2

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Variational Method  
Harmonic Oscillator



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# 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

$$\tilde{\psi} = \frac{1}{x^2 + a^2}$$

With this,

$$\langle \tilde{\psi} | \tilde{\psi} \rangle = \int_{-\infty}^{\infty} \left( \frac{1}{x^2 + a^2} \right)^2 dx$$



# Harmonic Oscillator

If we let

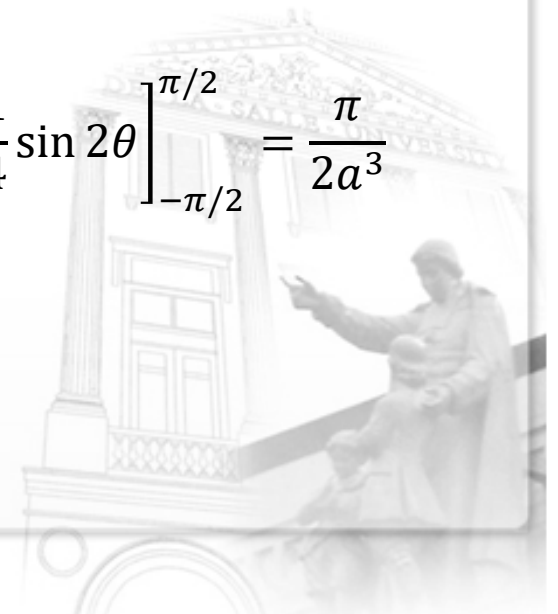
$$x = a \tan \theta$$

$$dx = a \sec^2 \theta d\theta$$

$$\left( \frac{1}{x^2 + a^2} \right)^2 dx = \frac{a \sec^2 \theta d\theta}{(a^2 \tan^2 \theta + a^2)^2} = \frac{\sec^2 \theta d\theta}{a^3 \sec^4 \theta} = \frac{1}{a^3} \cos^2 \theta d\theta$$

then

$$\langle \tilde{\psi} | \tilde{\psi} \rangle = \int_{-\infty}^{\infty} \left( \frac{1}{x^2 + a^2} \right)^2 dx = \frac{1}{a^3} \int_{-\pi/2}^{\pi/2} \cos^2 \theta d\theta = \frac{1}{a^3} \left[ \frac{\theta}{2} - \frac{1}{4} \sin 2\theta \right]_{-\pi/2}^{\pi/2} = \frac{\pi}{2a^3}$$



# Harmonic Oscillator

Now

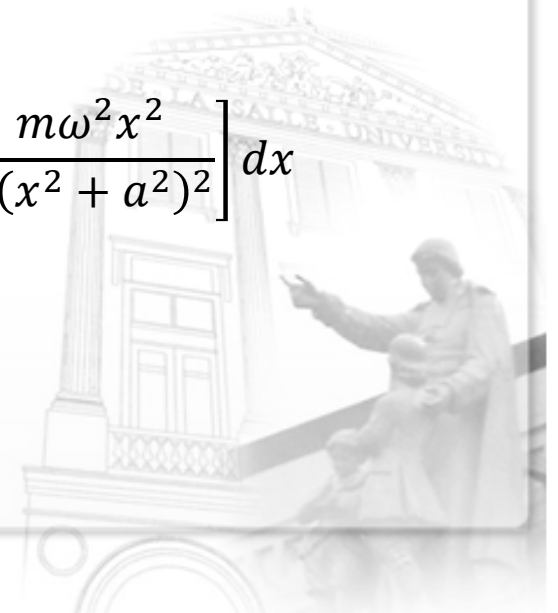
$$\frac{d^2}{dx^2} \left( \frac{1}{x^2 + a^2} \right) = \frac{d}{dx} \left( \frac{-2x}{(x^2 + a^2)^2} \right) = \frac{8x^2}{(x^2 + a^2)^3} - \frac{2}{(x^2 + a^2)^2}$$

Hence

$$H\tilde{\psi} = -\frac{\hbar^2}{2m} \left[ \frac{8x^2}{(x^2 + a^2)^3} - \frac{2}{(x^2 + a^2)^2} \right] + \frac{m\omega^2 x^2}{2(x^2 + a^2)}$$

and

$$\langle \tilde{\psi} | H | \tilde{\psi} \rangle = \int_{-\infty}^{\infty} \left[ -\frac{\hbar^2}{2m} \left[ \frac{8x^2}{(x^2 + a^2)^4} - \frac{2}{(x^2 + a^2)^3} \right] + \frac{m\omega^2 x^2}{2(x^2 + a^2)^2} \right] dx$$



# Harmonic Oscillator

With

$$x = a \tan \theta$$
$$dx = a \sec^2 \theta d\theta$$

We have

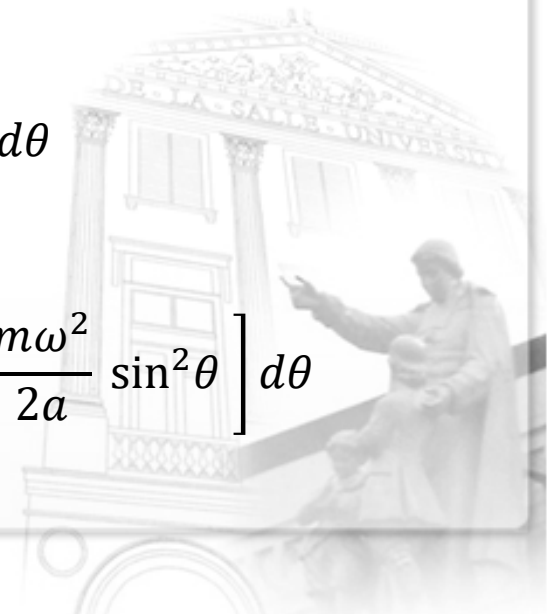
$$\frac{8x^2 dx}{(x^2 + a^2)^4} = \frac{8a^3 \tan^2 \theta \sec^2 \theta d\theta}{a^8 \sec^8 \theta} = \frac{8 \sin^2 \theta d\theta}{a^5 \sec^4 \theta} = \frac{8}{a^5} \sin^2 \theta \cos^4 \theta d\theta$$

$$\frac{2dx}{(x^2 + a^2)^3} = \frac{2a \sec^2 \theta d\theta}{a^6 \sec^6 \theta} = \frac{2}{a^5} \cos^4 \theta d\theta$$

$$\frac{x^2 dx}{(x^2 + a^2)^2} = \frac{a^3 \tan^2 \theta \sec^2 \theta d\theta}{a^4 \sec^4 \theta} = \frac{1}{a} \sin^2 \theta d\theta$$

and

$$\langle \tilde{\psi} | H | \tilde{\psi} \rangle = \int_{-\pi/2}^{\pi/2} \left[ -\frac{\hbar^2}{2m} \left[ \frac{8}{a^5} \sin^2 \theta \cos^4 \theta - \frac{2}{a^5} \cos^4 \theta \right] + \frac{m\omega^2}{2a} \sin^2 \theta \right] d\theta$$



# Harmonic Oscillator

Now

$$\frac{8}{a^5} \sin^2 \theta \cos^4 \theta - \frac{2}{a^5} \cos^4 \theta = \left[ \frac{8}{a^5} (1 - \cos^2 \theta) - \frac{2}{a^5} \right] \cos^4 \theta = \frac{6}{a^5} \cos^4 \theta - \frac{8}{a^5} \cos^6 \theta$$

Using the general formula

$$\cos^{2n} \theta = \frac{1}{2^{2n}} \binom{2n}{n} + \frac{1}{2^{2n-1}} \left\{ \cos 2n\theta + \binom{2n}{1} \cos(2n-2)\theta + \dots + \binom{2n}{n-1} \cos 2\theta \right\}$$

We have

$$\begin{aligned} \cos^4 \theta &= \frac{3}{8} + \frac{1}{2} \cos 2\theta + \frac{1}{8} \cos 4\theta \\ \cos^6 \theta &= \frac{5}{16} + \frac{15}{32} \cos 2\theta + \frac{3}{16} \cos 4\theta + \frac{1}{32} \cos 6\theta \end{aligned}$$

We also have

$$\sin^2 \theta = \frac{1}{2} - \frac{1}{2} \cos 2\theta$$



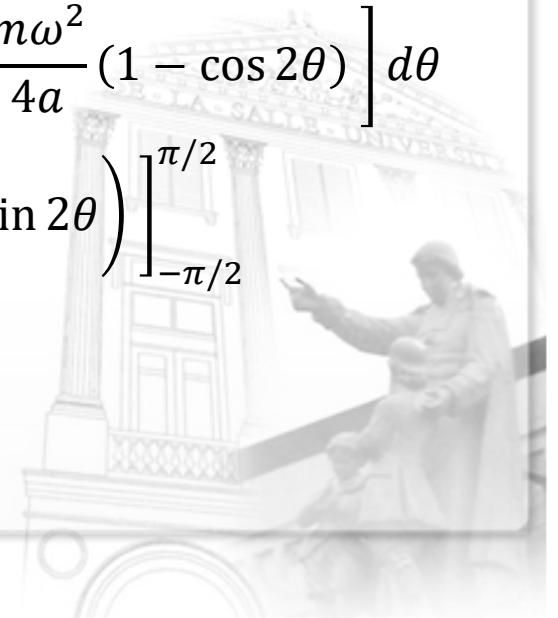
# Harmonic Oscillator

Hence

$$\begin{aligned} & \frac{8}{a^5} \sin^2 \theta \cos^4 \theta - \frac{2}{a^5} \cos^4 \theta \\ &= \frac{1}{a^5} \left[ \frac{9}{4} + 3 \cos 2\theta + \frac{3}{4} \cos 4\theta - \frac{5}{2} - \frac{15}{4} \cos 2\theta - \frac{3}{2} \cos 4\theta - \frac{1}{4} \cos 6\theta \right] \\ &= \frac{1}{a^5} \left[ -\frac{1}{4} - \frac{3}{4} \cos 2\theta - \frac{3}{4} \cos 4\theta - \frac{1}{4} \cos 6\theta \right] \end{aligned}$$

and

$$\begin{aligned} \langle \tilde{\psi} | H | \tilde{\psi} \rangle &= \int_{-\pi/2}^{\pi/2} \left[ \frac{\hbar^2}{8ma^5} (1 + 3 \cos 2\theta + 3 \cos 4\theta + \cos 6\theta) + \frac{m\omega^2}{4a} (1 - \cos 2\theta) \right] d\theta \\ &= \left[ \frac{\hbar^2}{8ma^5} \left( \theta + \frac{3}{2} \sin 2\theta + \frac{3}{4} \sin 4\theta + \frac{1}{6} \sin 6\theta \right) + \frac{m\omega^2}{4a} \left( \theta - \frac{1}{2} \sin 2\theta \right) \right]_{-\pi/2}^{\pi/2} \\ &= \frac{\hbar^2 \pi}{8ma^5} + \frac{m\omega^2 \pi}{4a} \end{aligned}$$



# Harmonic Oscillator

We thus have

$$\bar{H} = \frac{\langle \tilde{\psi} | H | \tilde{\psi} \rangle}{\langle \tilde{\psi} | \tilde{\psi} \rangle} = \frac{\hbar^2}{4ma^2} + \frac{1}{2}m\omega^2 a^2$$

To optimize, we set

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

This translates to

$$-\frac{\hbar^2}{2ma^3} + m\omega^2 a = 0$$

which gives

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





# Harmonic Oscillator

Our best estimate for the oscillator ground state energy using the trial function

$$\tilde{\psi} = \frac{1}{x^2 + a^2}$$

is therefore

$$\bar{H} = \frac{\sqrt{2}\hbar\omega}{4} + \frac{\hbar\omega}{2\sqrt{2}} = \frac{\hbar\omega}{\sqrt{2}}$$

Note that this is higher than the actual ground state energy  $\frac{\hbar\omega}{2}$ . The error of our estimate is

$$\frac{\frac{\hbar\omega}{\sqrt{2}} - \frac{\hbar\omega}{2}}{\frac{\hbar\omega}{2}} = \sqrt{2} - 1 = 41.4\%$$

This just goes to show that the choice of trial function matters a lot.

