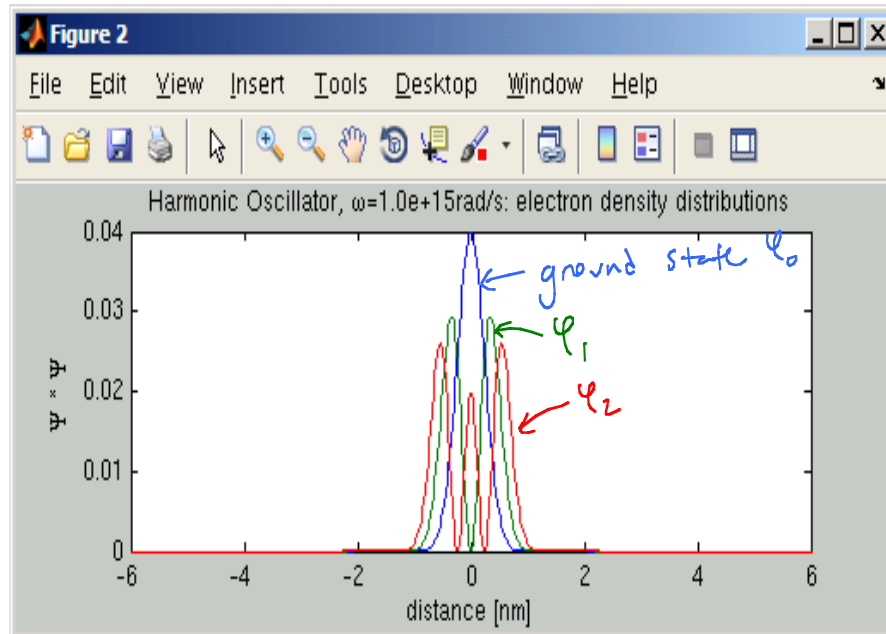
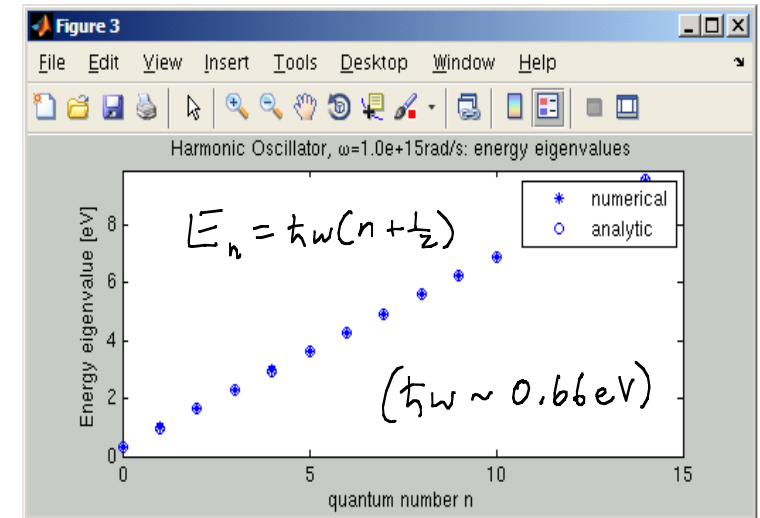
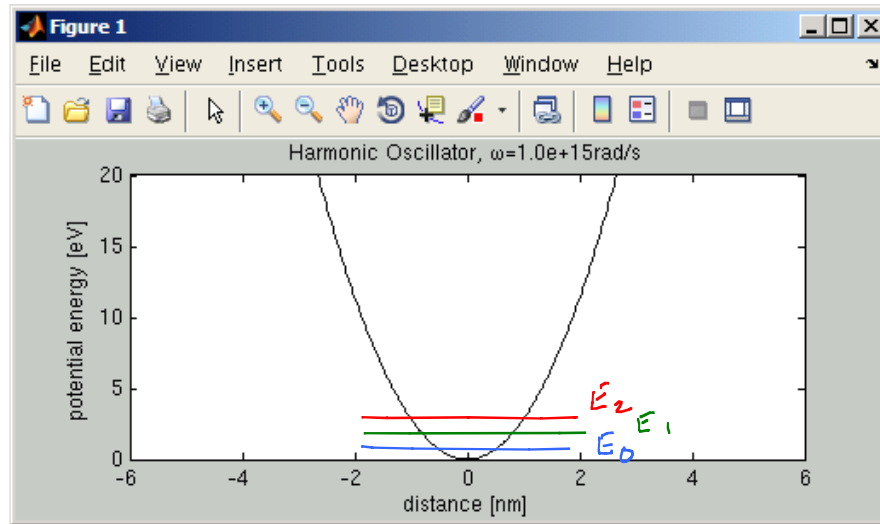


# Numerical solution to Harmonic oscillator



Notice that the probability density  $\psi^* \psi$  is confined to the bottom of the well, decays into classically forbidden region, and acquires more nodes (where  $\psi^* \psi = 0$ ) as  $n$  increases.

## Ground State properties from Heisenberg uncertainty rel'n

Energy of a wavefunction is determined by the expectation value of Hamiltonian

for Harmonic Oscillator  $\langle H \rangle = \frac{\langle p^2 \rangle}{2m} + \frac{1}{2} m \omega^2 \langle x^2 \rangle$ .

Since  $\langle p \rangle = 0$  for bound state and  $\langle x \rangle = 0$  for symmetric potential,

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \rightarrow \langle x^2 \rangle = \Delta x^2 \quad \text{and} \quad \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \rightarrow \langle p^2 \rangle = \Delta p^2$$

So  $\langle H \rangle = \frac{\Delta p^2}{2m} + \frac{1}{2} m \omega^2 \Delta x^2$  but we don't know either  $\Delta x$  or  $\Delta p$ .

However, we know the two are connected by the Heisenberg rel'n:

$$\Delta x \Delta p \geq \frac{\hbar}{2}, \quad \text{Using } \Delta p \geq \frac{\hbar}{2\Delta x}, \quad \text{we have}$$

$$\langle H \rangle \leq \frac{\hbar^2}{8m\Delta x^2} + \frac{1}{2} m \omega^2 \Delta x^2$$

The ground-state energy must be lower than the minimum value of the RHS.

## Minimization

$$\frac{d}{d\Delta X} \left( \frac{\hbar^2}{8m\Delta X^2} + \frac{1}{2}m\omega^2\Delta X^2 \right) = -\frac{\hbar^2}{4m\Delta X^3} + m\omega^2\Delta X = 0 \quad \text{which has sol'n } \Delta X = \sqrt{\frac{\hbar}{2m\omega}}$$

Let's compare to the exact solution  $\psi_0 \propto e^{-\frac{m\omega x^2}{2\hbar}}$ !

probability density  $\psi_0^* \psi_0 \propto e^{-\frac{m\omega x^2}{\hbar}} = e^{-\frac{x^2}{2\Delta X^2}}$  where  $\Delta X = \sqrt{\frac{\hbar}{2m\omega}}$

Same!

We can also calculate the upper bound on energy of the ground state:

$$\langle H \rangle \leq \frac{\hbar^2}{8m\Delta X^2} + \frac{1}{2}m\omega^2\Delta X^2 = \frac{\hbar^2}{8m\frac{\hbar}{2m\omega}} + \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega} = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

Same as analytical value for  $E_0$ !

In this case, the inequality is an equality because the gaussian ground state minimizes the product  $\Delta x \Delta p$ !

In general, of course, ground state wavefunctions are not gaussian and this procedure only gives an upper bound.