March 4, 2021

Quantum Harmonic Oscillator

Hooke's law $F = -kx$ can be integrated to find the potential energy, $V(x) = kx^2/2 = m\omega^2 x^2/2$, stored in a spring. Substituting this potential into the 1D TISE gives the differential equation

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\,\omega^2 x^2 \psi(x) = E\,\psi(x).} \tag{1}$$

To solve, the first step is to make the substitution $x = y\,a$, where $a = \sqrt{\frac{\hbar}{m\,\omega}}$. This creates a dimensionless differential equation

$$\boxed{\frac{d^2\psi(y)}{dy^2} + (\varepsilon - y^2)\psi(y) = 0,} \tag{2}$$

with "dimensionless energy" $\varepsilon = E/(\hbar\omega/2)$.
The boundary conditions are: when $y \to \pm\infty$ then $\psi(y) \to 0$.
It is found that solutions of the form $\psi(y) = y^n e^{-y^2/2}$ are solutions in the limit of large y, where $e^{-y^2/2}$ is a Gaussian.

Equation 2 is solved properly in PH2130; the eigenfunctions and energies are

$$\psi_n(y) = H_n(y)\,e^{-\frac{y^2}{2}} \quad \text{and} \quad \varepsilon = (2n+1) \tag{3}$$

where $H_n(y)$ are the Hermite polynomials. $H_n(y)$ are even (odd) functions of y if n is an even (odd) integer.

Converting back to the variable x we have normalised wavefunctions and energies:

$$\psi_n(x) = \frac{H_n(x/a)}{\sqrt{2^n\,n!\,\sqrt{\pi\,a^2}}}\,e^{-\frac{x^2}{2a^2}} \quad \text{and} \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \tag{4}$$

which for $n = 0, 1, 2, 3$ and 4 are given in the following table:

n	$H_n(y)$	$\psi_n(x)$
0	1	$\psi_0(x) = \frac{1}{\sqrt[4]{\pi a^2}}\, e^{-\frac{x^2}{2a^2}}$
1	$2y$	$\psi_1(x) = \frac{\sqrt{2}\,(x/a)}{\sqrt[4]{\pi a^2}}\, e^{-\frac{x^2}{2a^2}}$
2	$4y^2 - 2$	$\psi_2(x) = \frac{[4(x/a)^2-2]}{2\sqrt{2}\,\sqrt[4]{\pi a^2}}\, e^{-\frac{x^2}{2a^2}}$
3	$8y^3 - 12y$	$\psi_3(x) = \frac{[8(x/a)^3-12(x/a)]}{4\sqrt{3}\,\sqrt[4]{\pi a^2}}\, e^{-\frac{x^2}{2a^2}}$
4	$16y^4 - 48y^2 + 12$	$\psi_4(x) = \frac{[16(x/a)^4-48(x/a)^2+12]}{8\sqrt{6}\,\sqrt[4]{\pi a^2}}\, e^{-\frac{x^2}{2a^2}}$

- The wavefunctions are orthogonal and normalised:

$$\int_{-\infty}^{\infty} \psi_m^*(x)\, \psi_n(x)\, dx = \langle \psi_m | \psi_n \rangle = \delta_{nm}. \tag{5}$$

- Figure 1 shows plots of $\psi_n(y)$.

- The lowest energy state, the ground state, is given by $n = 0$. The zero-point energy is $\hbar\omega/2$.

- The normalised ground state wavefunction is $\psi_0(x) = \frac{1}{(\pi a^2)^{1/4}}\, e^{-\frac{x^2}{2a^2}}$, from which we can calculate $\Delta x = \frac{a}{\sqrt{2}}$ and $\Delta p = \frac{\hbar}{\sqrt{2}a}$; we find that $\Delta p\, \Delta x = \frac{\hbar}{2}$. Note the uncertainty principle is usually written as

$$\Delta p\, \Delta x \geq \frac{\hbar}{2}, \tag{6}$$

  the minimum value is obtained with a Gaussian wavefunction of the ground state. This comes from the fact that Gaussians minimise uncertainties, something you should know from PH2130.

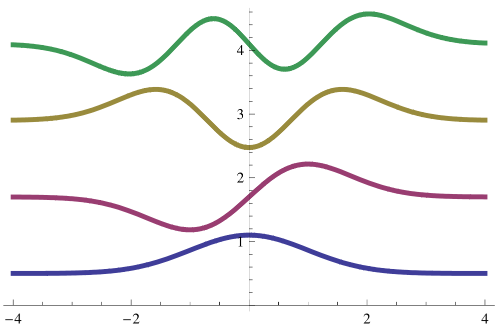

Figure 1: The four lowest energy wavefunctions $\psi_n(y) = H_n(y)\, e^{-\frac{y^2}{2}}$ in a harmonic well, plotted as a function of $y = x/a$.

The uncertainties in position and momentum, Δx and Δp, are given by

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \tag{7}$$

and

$$(\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2. \tag{8}$$

Exercises

1. The ground state wave function is $\psi_0(x) = \frac{1}{(\pi a^2)^{1/4}}\, e^{-\frac{x^2}{2a^2}}$. Plot $\psi_0(x)$ and the probability density $p(x) = |\psi_0(x)|^2$. Set $a = 1$ in the plots, and label the horizontal axis as x/a. Note the symmetry (is it odd or even) of the two plots.

2. Show that the ground state wavefunction is normalised, and is orthogonal to ψ_1, ψ_3, ψ_4 and ψ_7. That is, show that it follows the general expression

$$\int_{-\infty}^{\infty} \psi_0^*(x)\, \psi_n(x)\, dx = \langle \psi_0 | \psi_n \rangle = \delta_{0n}. \tag{9}$$

   This is a good check of the accuracy of your numerical integrations, which can be done using `quad` in the `scipy.integrate` module (see Week 8 of the PH2150 course).

3. Do a numerical integration to show that

$$\int_{-\infty}^{\infty} \psi_0^*(x)\, x\, \psi_0(x)\, dx = \langle \psi_0 |\, x\, | \psi_0 \rangle = 0. \tag{10}$$

   Is this result consistent with the symmetry of $|\psi_0(x)|^2$.

   Show that $\langle \psi_0 | p | \psi_0 \rangle = 0$, remembering that $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$. In one dimension, then $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$.
   Numerical differentiations can be done using `derivative` in the `scipy.misc.derivative` module. Call the function using `dx=0.0001`, and the second order derivative can be obtained with a single call by specifying `n=2` (not to be confused with the n in ψ_n).

4. Do a numerical integration to show that

$$\int_{-\infty}^{\infty} \psi_0^*(x)\, x^2\, \psi_0(x)\, dx = \langle \psi_0 |\, x^2\, | \psi_0 \rangle = a^2/2. \tag{11}$$

5. Do a numerical integration to show that

$$\int_{-\infty}^{\infty} \psi_0^*(x)\, p^2\, \psi_0(x)\, dx = -\hbar^2 \langle\psi_0|\, \frac{d^2}{dx^2}\, |\psi_0\rangle = \frac{\hbar^2}{2a^2}. \tag{12}$$

6. Hence show that for the ground state, $n = 0$, in a quantum harmonic oscillator

$$\Delta x = \frac{a}{\sqrt{2}} \quad \text{and} \quad \Delta p = \frac{\hbar}{\sqrt{2}a},$$

and the uncertainty relation gives

$$\Delta x\, \Delta p = \frac{\hbar}{2}. \tag{13}$$

7. Calculate and tabulate Δx, Δp, and $\Delta x\, \Delta p$ for $n = 0 - 10$. By observation work out the general expression for these quantities as a function of n.

8. Use the previous results (and some simple algebra) to show that the expectation values for the kinetic energy and potential energy,

$$\left\langle \frac{p^2}{2\,m} \right\rangle \quad \text{and} \quad \left\langle \frac{m\,\omega^2\, x^2}{2} \right\rangle,$$

are both equal to $\frac{\hbar\,\omega}{4}(2n+1)$.

9. The probability density for the classical harmonic oscillator with amplitude a is given by

$$p(x) = \frac{1}{\pi\sqrt{a^2 - x^2}}, \tag{14}$$

for $|x| < a$. In accordance with Bohr's correspondence principle, show that the quantum solutions $|\psi_n(x)|^2$ tend to this result as n becomes very large.

The link below maybe a useful starting point for your coding:
`https://chem.libretexts.org/Ancillary_Materials/Interactive_Applications/Jupyter_Notebooks/Quantum_Harmonic_Oscillators_-_Plotting_Eigenstates_(Python_Notebook)`